# TOPIC 10. STRUCTURE DETERMINATION

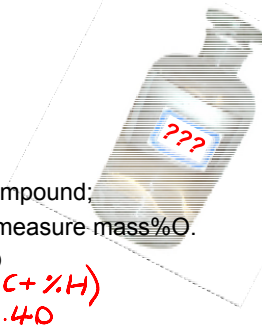
## OBJECTIVES

1. Use combustion analysis to determine empirical formula.
2. Determine molecular weight (and molecular formula) from mass spectrometry.
2. Calculate number of rings and double bonds from molecular formula.
3. Determine functional groups present from infrared spectroscopy.
4. Use $^{1}H$ and $^{13}C$ NMR spectroscopy to identify other structural features.
5. Combine conclusions from individual techniques to determine the structure of organic compounds.

*Problems in this section will be restricted to the following classes of aliphatic and aromatic compounds:*

Alkanes, alkenes, alkynes, alkyl halides, alcohols, ethers, aldehydes, ketones, carboxylic acids, esters, acyl chlorides, anhydrides, amides, amines, nitriles

# COMBUSTION ANALYSIS




$$C_xH_yO_z + O_2 \longrightarrow xCO_2 + (y/2)H_2O$$

Measure mass of $CO_2$ and $H_2O$ formed from a known mass of compound; data cited as mass% of each element present. Generally do not measure mass%O.

| *e.g.*, | C | H | O |
|---|---|---|---|
| Mass% | 54.51 | 9.09 | 100 − (%C + %H) = 36.40 |
| Mole Ratio | $\frac{54.51}{12.01}$ | $\frac{9.09}{1.01}$ | $\frac{36.40}{16.00}$ |
| = | 4.539 | 9.00 | 2.275 |
| = | 1.995 | 3.96 | 1.000 |

= *Empirical formula*

Be careful when rounding, elemental analyses provided ±0.4 mass% - do not round by more than 0.05 to 0.1. Multiply ratios *before* rounding.

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# EMPIRICAL AND MOLECULAR FORMULAS; DETERMINATION OF "SODAR"

Molecular formula is an integral number of times the empirical formula.

$C_2H_4O$

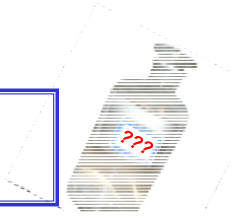
Sum of double bonds and rings ("SODAR")

*For C,H,O: (2#C + 2 – #H) / 2*

*For C,H,O,N,Hal: (2#C + 2– #H – #Hal + #N) / 2*

*Each Hal replaces a H*
*Each N adds an extra H*
*S,O: no effect on calculation*

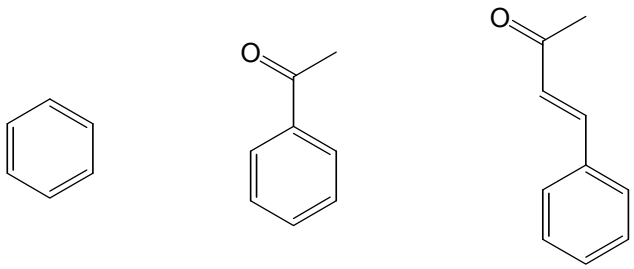
If SODAR calculated from empirical formula is not a positive integral (or 0), this cannot be the molecular formula.




$C_2H_4O$

| MOLECULAR FORMULA COULD BE: |
|---|
| |

*If SODAR ≥4*: consider the possible presence of a benzene ring

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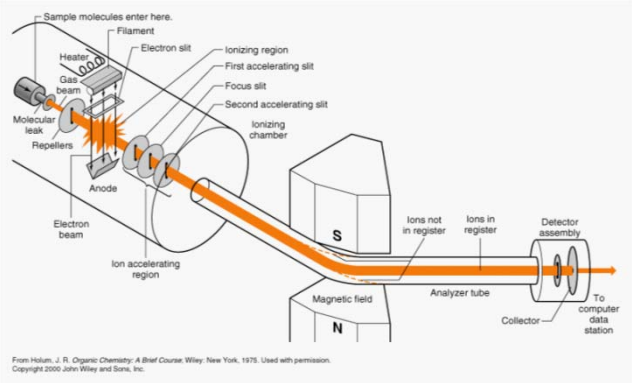
# MASS SPECTROMETRY

## Theory and Experiment

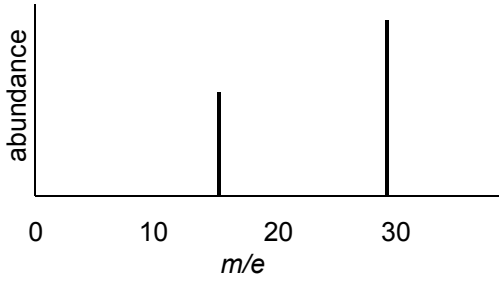



$M + e^- (70\ eV) \longrightarrow M^+ + 2e^-$

$M^+ \longrightarrow$ lower mass ions

## Data Available

*e.g.*, mass spectrum of ethane, $CH_3CH_3$




Ions also fragment, which can give further clues about the structure (beyond scope of this course).

Knowledge of molecular weight (from mass spec) and empirical formula (from combustion analysis) allows determination of molecular formula.

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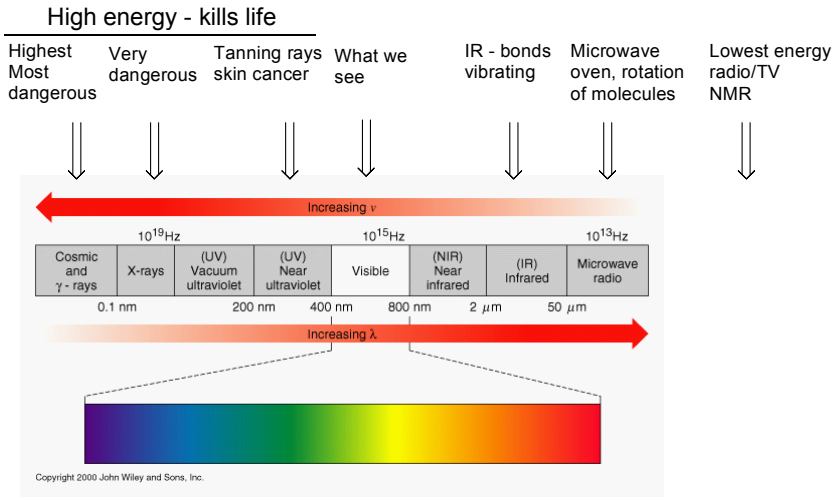
Empirical formula: $C_2H_4O$

Mass spectrum: $M^+$ *m/e* = 88


MOLECULAR FORMULA **IS**:

# SPECTROSCOPY:
# THE INTERACTION OF LIGHT AND MATTER

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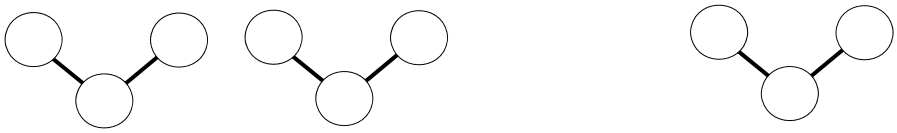
# INFRARED SPECTROSCOPY

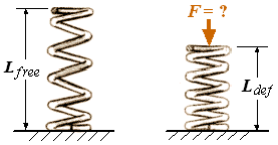
## Molecular Vibrations: Stretching and Bending



*Analogy to masses and springs:*

Spring constant (strength) ↑, Frequency, $\upsilon$

Masses ↑ , $\upsilon$



## Electromagnetic Radiation

$E = h\nu$ $\quad$ $c = \lambda\nu$

For molecular vibrations,

Frequency, $\nu$ = 6 x $10^{12}$ to 1.25 x $10^{14}$ Hz

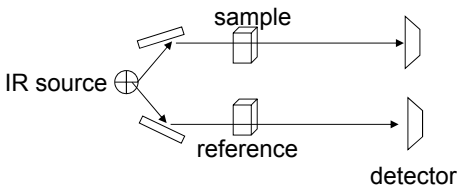
Wavelength, $\lambda$ = 50 to 2.5 $\mu$m

Define wavenumber, $\bar{\nu} = \dfrac{1}{\lambda(\text{in cm})}$

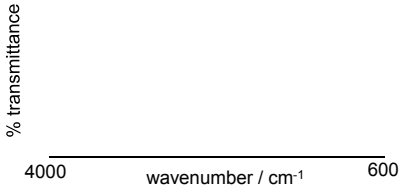
= *200 to 4000 $cm^{-1}$*

## Instrumentation

A simple scheme




## Spectrum

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## Selected Infrared Absorptions

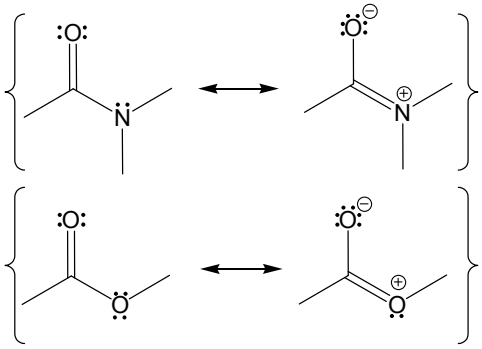
| **Functional Group** | **Range $cm^{-1}$** | **Intensity and shape** |
|---|---|---|
| $sp^3C$—H | 2850-2960 | medium to strong; sharp |
| $sp^2C$—H | 3010-3190 | medium to strong; sharp |
| spC—H | about 3300 | medium to strong; sharp |
| C═C | 1620-1660 | weak to medium; sharp |
| C≡C | 2100-2260 | weak to medium; sharp |
| N—H | 3300-3500 | medium; *broad* |
| O—H (very dilute) | about 3600 | medium; sharp |
| O—H (H-bonded) | 3200-3550 | strong; *broad* |
| O—H (carboxylic acid) | 2500-3000 | medium; *very broad* |
| C—O | 1050-1150 | medium to strong; sharp |
| C═O (aldehyde,ketone) | 1690-1740 | very strong; sharp |
| C═O (ester) | 1735-1750 | very strong; sharp |
| C═O (carboxylic acid) | 1710-1780 | strong; sharp |
| C═O (amide) | 1630-1690 | strong; sharp |
| C≡N | 2200-2260 | medium; sharp |

*Validating resonance theory*

C=O (ester) 1735-1750 $cm^{-1}$
C=O (amide) 1630-1690 $cm^{-1}$

*Which is the stronger bond?*

*Can we understand this using resonance theory?*



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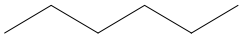
Infrared spectroscopy indicates the presence of particular bonds in a sample. The combination of bonds indicates which functional groups are present.

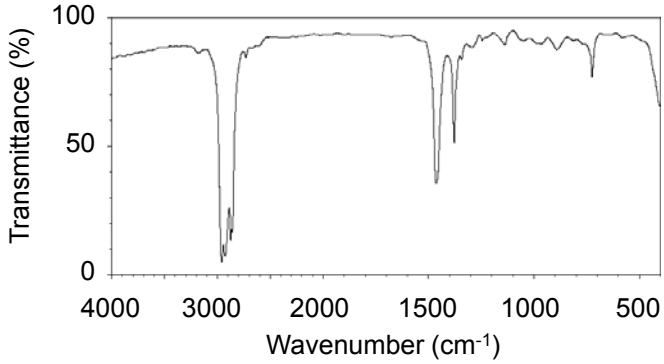
You do not need to memorize IR frequency data. However, you *must* develop experience at interpreting IR spectra to be able to determine the presence of particular functional groups.

| O-H | C=O | C-O | |
|---|---|---|---|
| ✓ | | ✓ | Alcohol |
| | | ✓ | Ether |
| | ✓ | | Aldehyde or ketone |
| | ✓ | ✓ | Ester |
| ✓ | ✓ | ✓ | Carboxylic acid |

4000 Wavenumber / $cm^{-1}$ 600

*Hexane*



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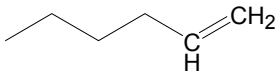
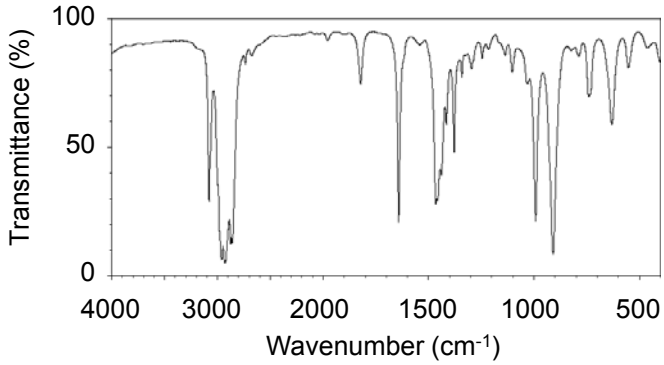
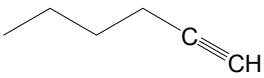
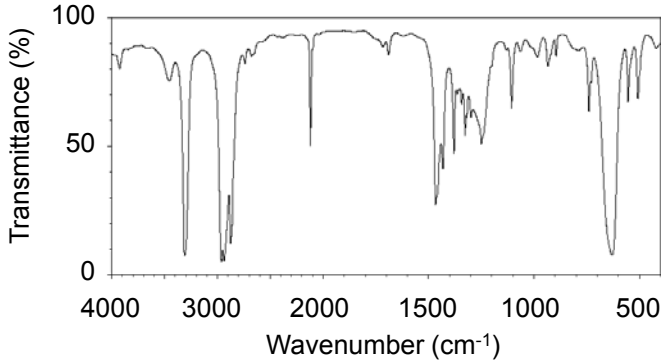
*1-Hexene*



*1-Hexyne*

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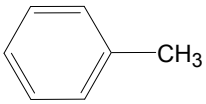
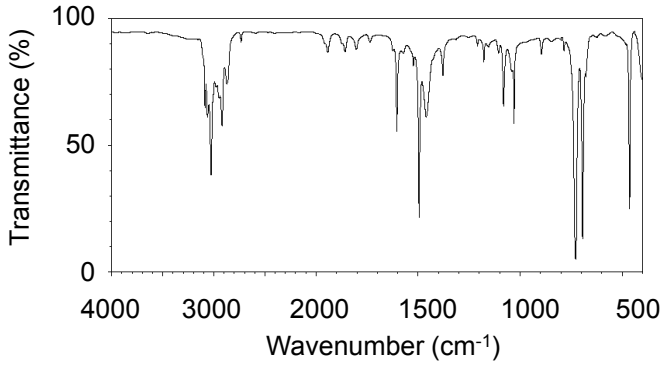
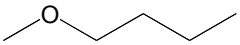
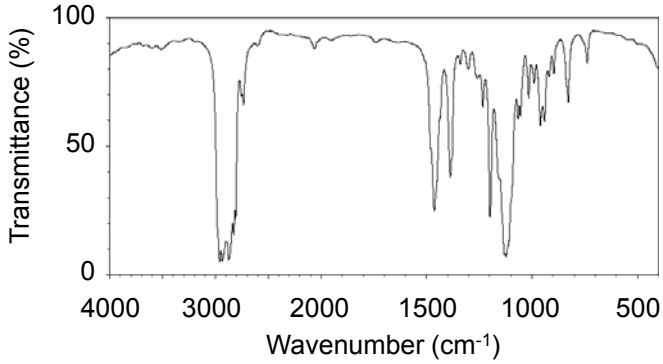
*Toluene*



*Butyl methyl ether*

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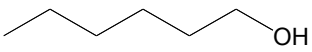
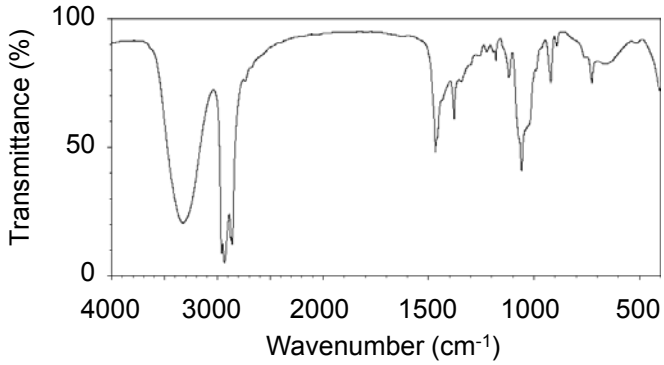
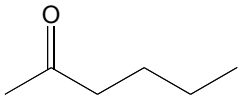
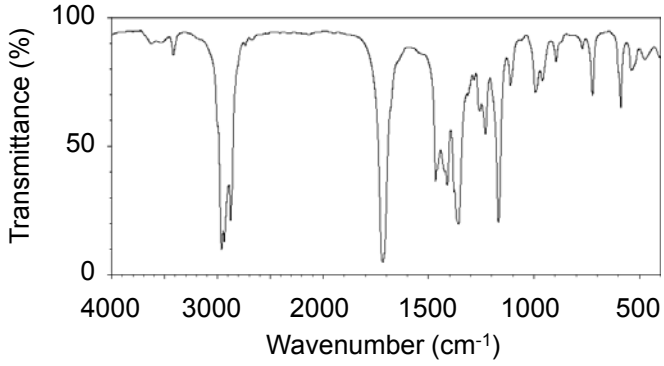
*1-Hexanol*



*2-Hexanone*

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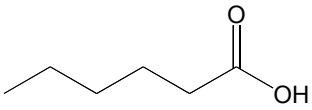
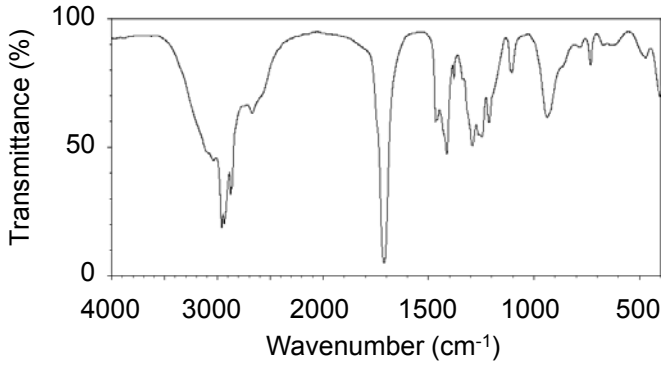
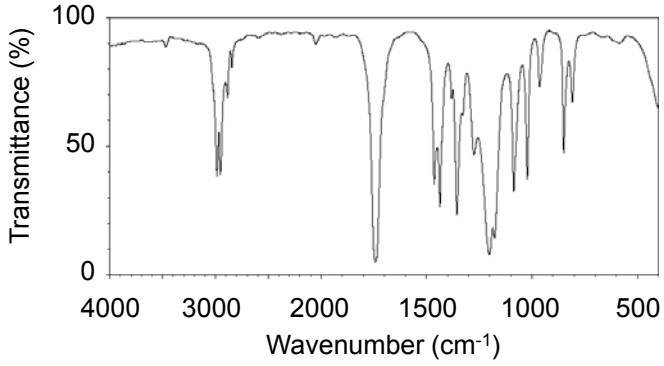
*Hexanoic Acid*



*Methyl Propionate*

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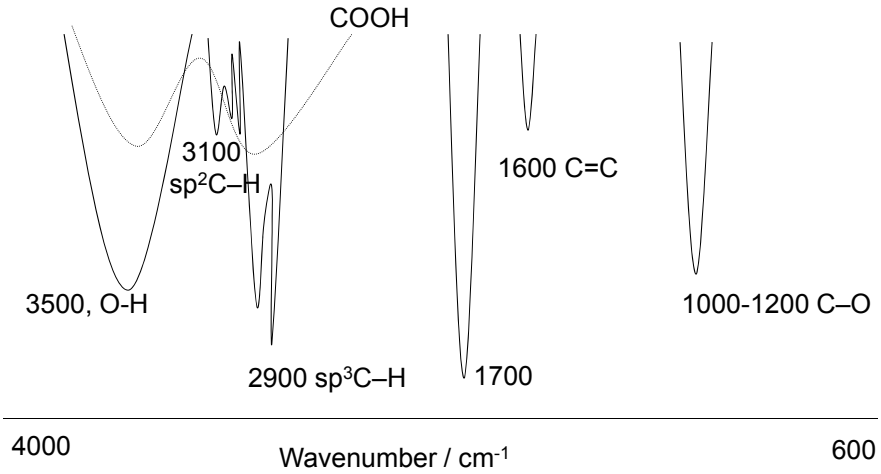
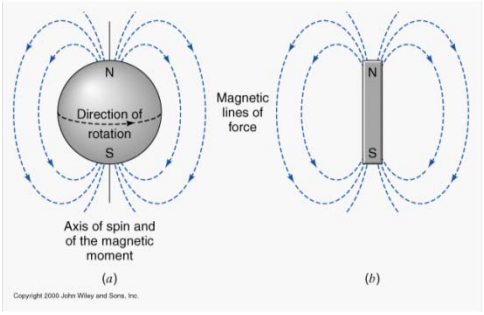
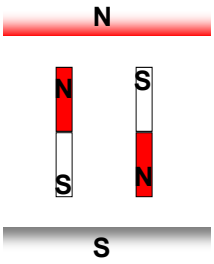
## Important infrared adsorptions

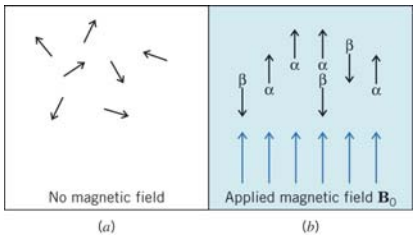


# HYDROGEN (PROTON) NUCLEAR MAGNETIC RESONANCE ($^1$H NMR) SPECTROSCOPY

## Nuclear Spin ($^1$H, $^{13}$C, $^{19}$F, $^{31}$P)

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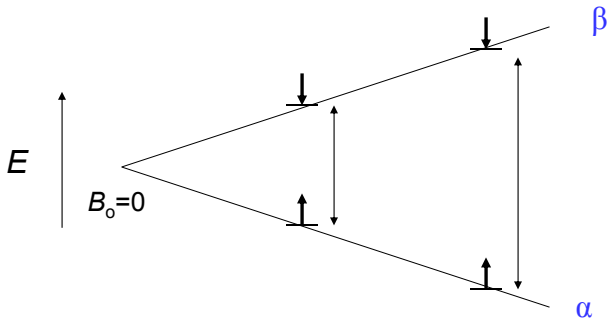
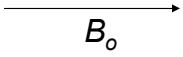
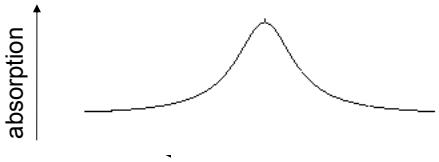
## The Energy of the Spin States of Hydrogen Nuclei in a Magnetic Field



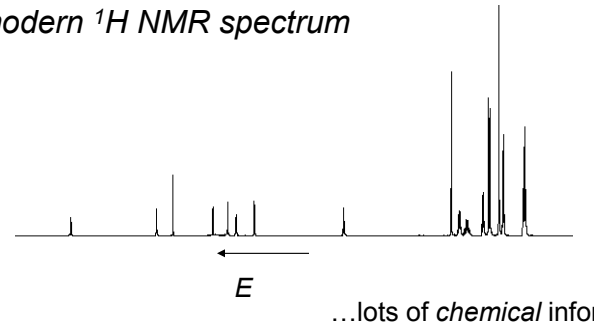

The frequency $\nu$ required to flip the spin state from α to β is called ***resonance frequency***

*An early $^1H$ NMR spectrum*




...not much *chemical* information

*A modern $^1H$ NMR spectrum*




…lots of *chemical* information

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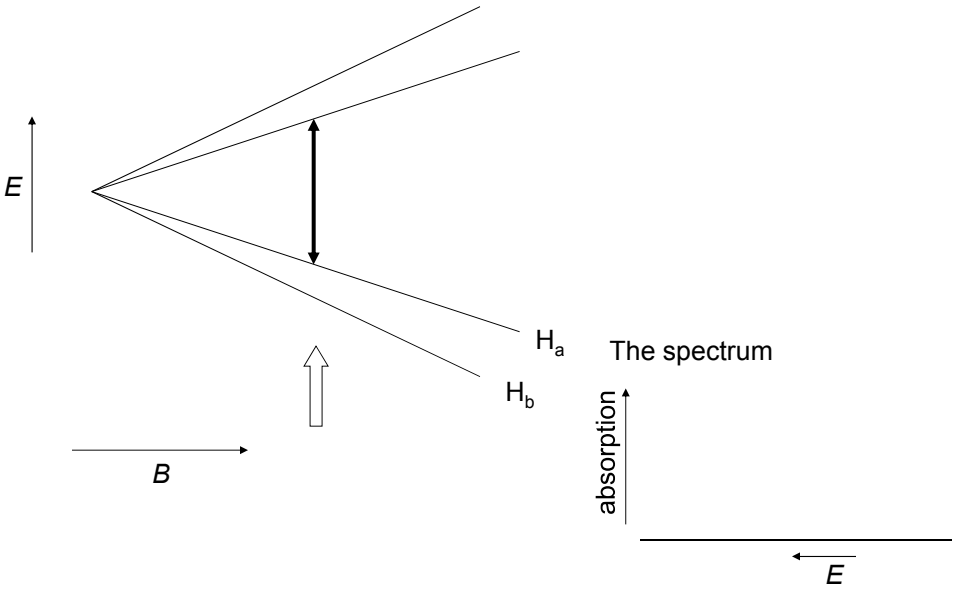
If the *applied magnetic field* is held constant, the protons $H_a$ and $H_b$ absorb irradiation with different frequencies.

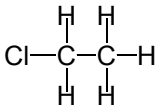


## Preview: Types of Information available from a $^1$H NMR spectrum

A $^1$H nuclear magnetic resonance spectrum contains information about the:

(a) number of different types of proton

(b) relative number of each type of proton



(c) proximity to functional groups

(d) the number of *adjacent* protons

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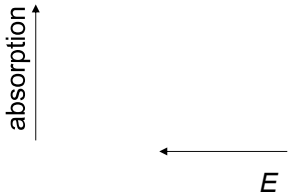
### (a) The number of signals in the spectrum is the number of types of proton.

$^1$H NMR spectrum of methane $CH_4$




one peak ⇒ one type of proton

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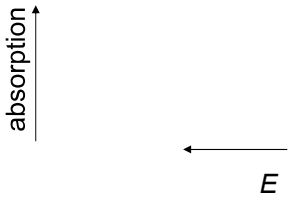
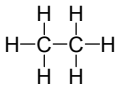
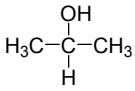
$^1$H NMR spectrum of ethane $CH_3–CH_3$

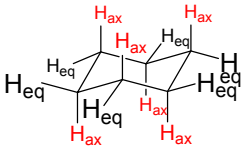



one peak ⇒ one type of proton

Protons that are related to each other by a rotation or plane of symmetry are identical (chemical shift equivalent)

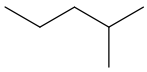


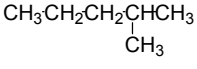


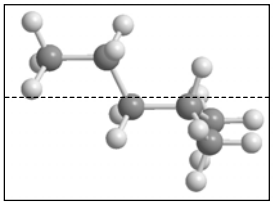


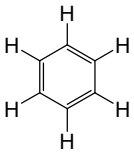

*low temperature:*
2 signals

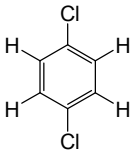
*high temperature (room T):*
1 averaged signal

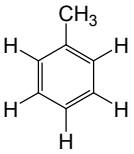


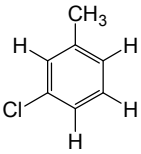












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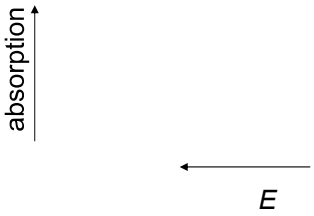
$^{1}$H nuclear magnetic resonance spectrum of methanol…

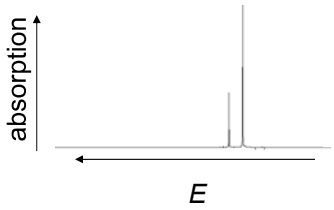
$CH_3$–OH




two peaks ⇒ two types of proton

## (b) The relative area of each peak (the integration) corresponds to the relative number of each type of proton

$^1$H NMR spectrum of methanol

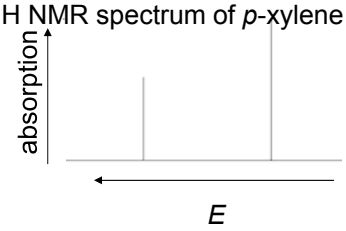


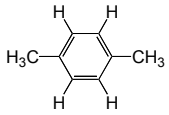

$H_3C{-}OH$

integral ratio __:__ ⇒ ratio of types of proton

---

$^1$H NMR spectrum of *p*-xylene



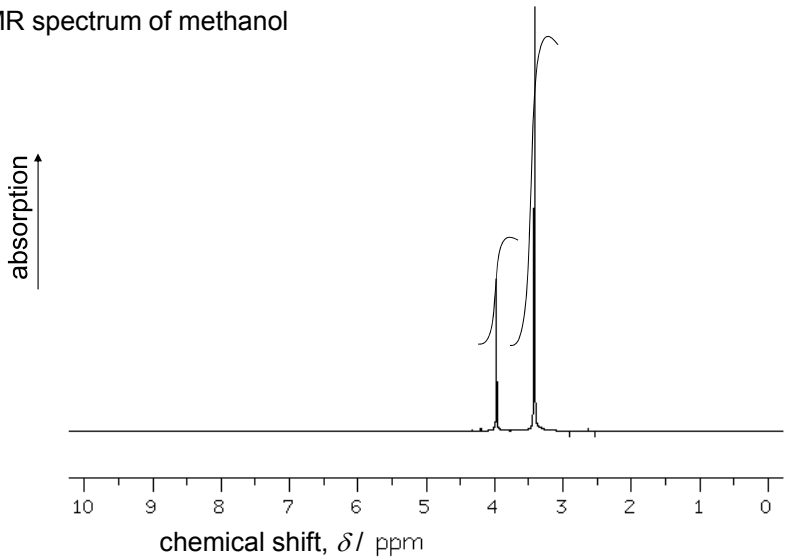




integral ratio __:__ ⇒ ratio of types of proton

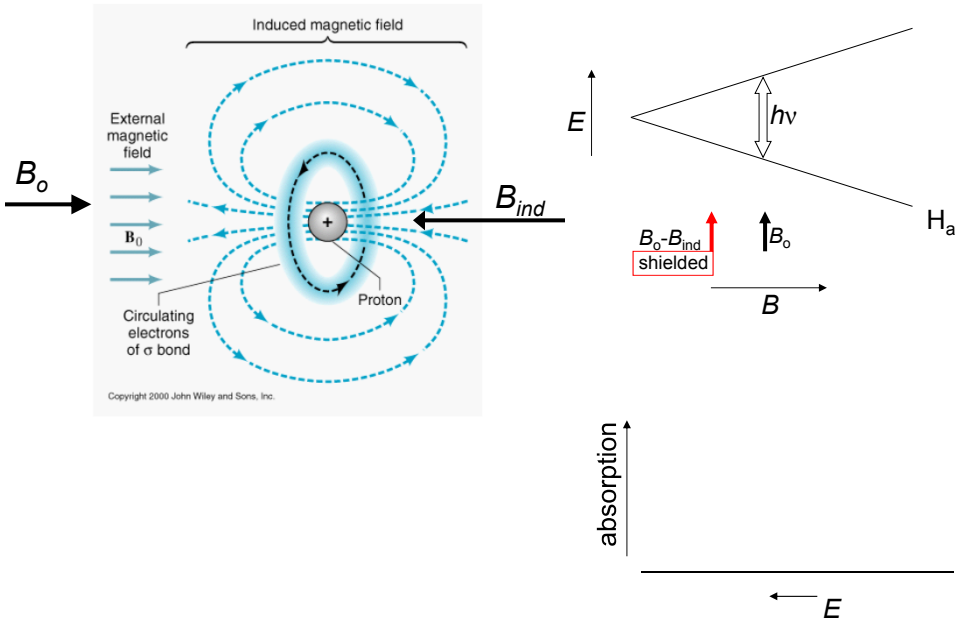
---

## (c) The chemical shift indicates the environment of the proton

$^1$H NMR spectrum of methanol



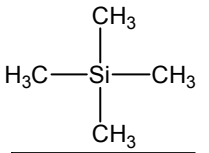
## *Shielding and Deshielding*




---

## *The δ-scale*

The frequency at which a proton resonates is measured relative to the frequency for the protons of tetramethylsilane, TMS (which resonates at a relatively low frequency), and cited on the δ (delta) scale in parts per million of the frequency at which TMS resonates.



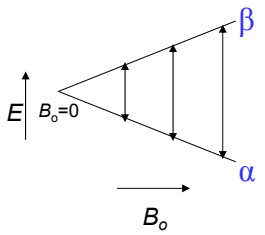

| electronegativity |
|---|
| C=2.5 |
| Si=1.7 |

$$\delta = \frac{\nu_{proton} - \nu_{TMS}}{\nu_{TMS}} \times 10^6 \quad [ppm]$$

e.g. $\nu_{TMS} = 300,000,000$ Hz (7T magnet)

$\nu_{Sample} = 300,000,617$ Hz

$$\delta = \frac{617}{300 \times 10^6} \times 10^6 = 2.06 \text{ ppm}$$





| Field Strength $B$ / T | $\upsilon_{TMS}$ / Hz | $\upsilon_{CH_4}$ / Hz | $\delta_{CH_4}$ / ppm |
|---|---|---|---|
| 2.33 | 100,000,000 | 100,000,100 | 1 |
| 4.66 | 200,000,000 | 200,000,200 | 1 |
| 7.00 | 300,000,000 | 300,000,300 | 1 |

- The *resonance frequency* (in Hz) depends on magnet strength.

- The *chemical shift* ($\delta$) is independent of magnet strength.

---

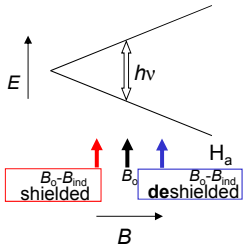
*Effect of Structure on Chemical Shift ($\delta$ scale, ppm)*

$CH_3$-$CH_3$ *0.9*

$CH_3$- $N(CH_3)_2$ *2.2*

$CH_3$-$OCH_3$ *3.2*

$CH_3$-F *4.3*




$CH_3$-Cl *3.1*

$CH_3$-Br *2.7*

$CH_3$-I *2.2*

$CHCl_3$ *7.3*

$CH_2Cl_2$ *5.3*

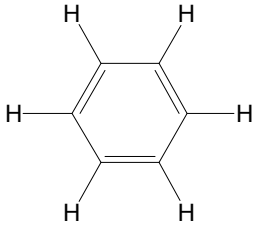
$CH_3Cl$ *3.1*

**Approximate [$^1$H]-NMR chemical shifts for various substitutent groups**

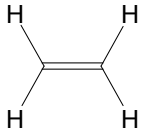
| Type of proton | Expected range Chemical shift (δ) |
|---|---|
| $(CH_3)_4Si$ | 0.00 |
| $CH_3$-C-R ($sp^3$) | 0.9 - 1.8 |
| -$CH_2$-C-R ($sp^3$) | 1.1 - 2.0 |
| -CH-C-R ($sp^3$) | 1.3 - 2.1 |
| H-C-N | 2.2 - 2.9 |
| H-C-O | 3.3 - 3.7 |
| H-C-Cl | 3.1 - 4.1 |
| H-C-Br | 2.7 - 4.1 |
| H-C-C=O | 2.1 - 2.5 |
| H-C-C=C | 1.6 - 2.6 |
| H-C-Ar | 2.3 -2.8 |
| H-C=O ($sp^2$) | 9 - 10 |
| H-C=C ($sp^2$) | 4.5 - 6.5 |
| H-Ar ($sp^2$) | 6.5 - 8.5 |
| H-C  C (sp) | 2.5 |
| H-N (amine) | 1 - 3 |
| H-OR (alcohol) | 0.5 - 5 |
| H-OAr (phenol) | 6 - 8 |
| H-$O_2$CR (acid) | 10 - 13 |

You will be provided with a copy of *Table 9.1* on exams. This provides *approximate* ranges for values of chemical shifts for particular types of protons. Remember that protons adjacent to two (or more) electron withdrawing groups will appear further downfield than a proton adjacent to only one.

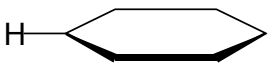
---

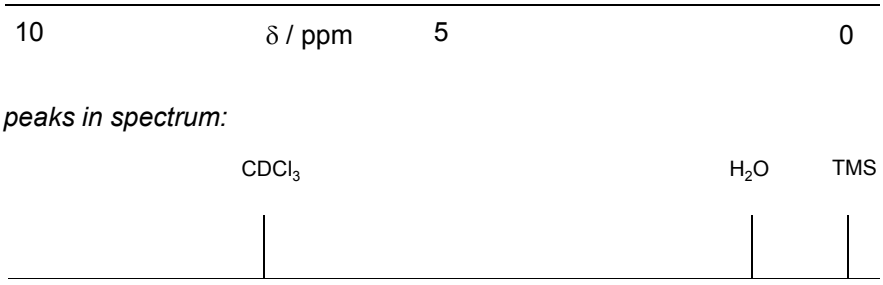



δ=7.3




δ=5.3

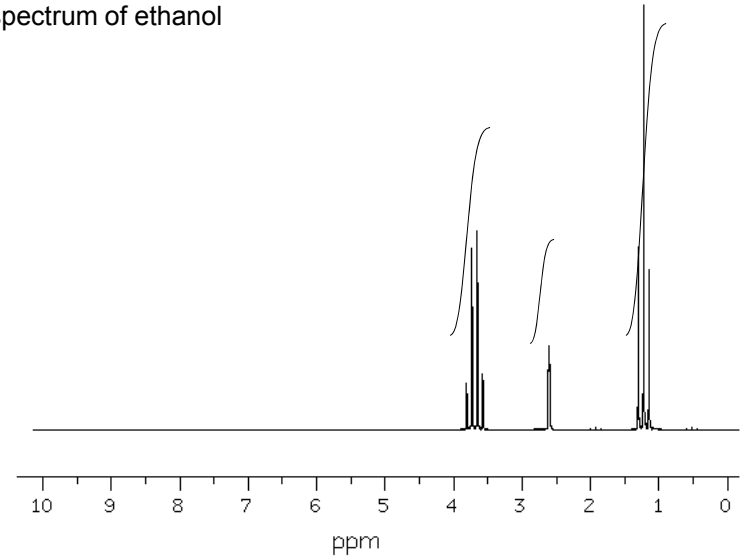





*Other peaks in spectrum:*

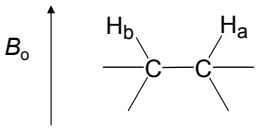
## (d) The multiplicity of a signal indicates the number of adjacent protons

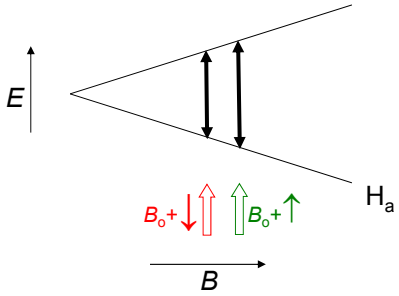
$^1$H NMR spectrum of ethanol



*Spin-Spin Coupling*

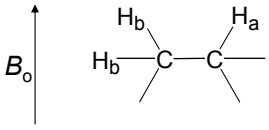
The magnetic field experienced by a proton is effected by the magnetic field generated by each adjacent proton.




If $H_b$ spin ↑, need to apply *larger E (=hν)* to achieve resonance of $H_a$
If $H_b$ spin ↓, need to apply *smaller E (=hν)* to achieve resonance of $H_a$

---




To achieve resonance of $H_a$
If $H_b$ spins ↑ + ↑, need to apply *higher* $\nu$
If $H_b$ spins ↑ + ↓, or, ↓ + ↑ signal appears at $\delta_a$
If $H_b$ spins ↓ + ↓, need to apply *lower* $\nu$

Coupling is only observed between *non-equivalent protons*.

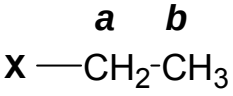
The signal for a proton with *N* adjacent *equivalent* protons will be split into a multiplet consisting of *N*+1 lines.

The relative area of each peak *within* a multiplet can be determined from Pascal's triangle

---

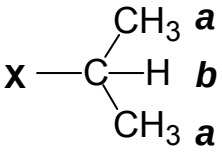
*Some Common Sets of Multiplets*

Et–X



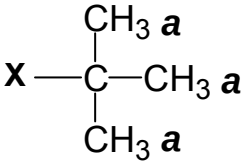

***a***
***b***

i-Pr–X

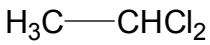



***a***
***b***

t-Bu–X




***a***



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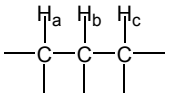
*Problems:* How can you get a pentet?

*Multiplets of Multiplets*

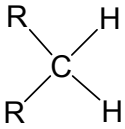



$J_{ab} = J_{bc}$

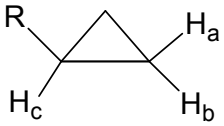
$J_{ab} > J_{bc}$

---

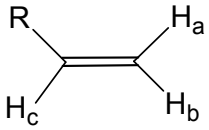
*Geminal protons*




Rings




Vinyl groups



## Summary: Types of information available from $^1$H NMR spectrum

| | |
|---|---|
| Number of signals | Number of *types* of proton |
| Integral of signals | *Relative number* of each type of proton |
| Chemical Shift | Electronic environment |
| Multiplicity | Number of *adjacent* protons |

---

*Problems:* Predict the appearance (chemical shift, integral and multiplicity) of the $^1$H NMR signals of the following compounds.

(a) 2-butanone, $CH_3COCH_2CH_3$

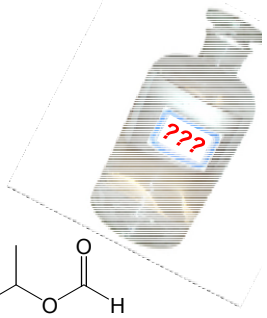
(b) methyl 3-chloropropanoate, $ClCH_2CH_2CO_2CH_3$

$C_4H_6O_2$

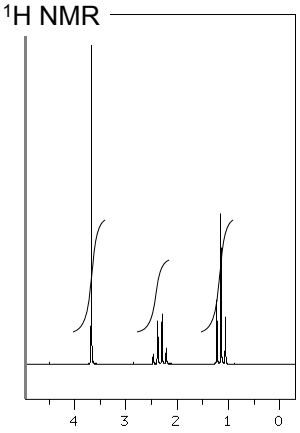
SODAR = 1

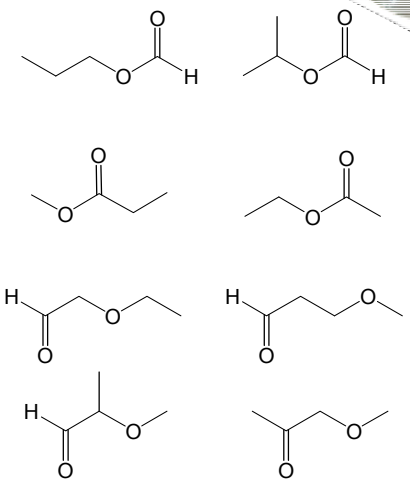
IR: 1720 $cm^{-1}$ » C=O

no peak at 3300 $cm^{-1}$ » no O-H




$^1$H NMR



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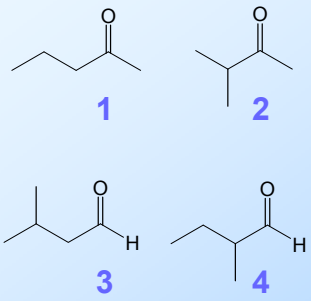
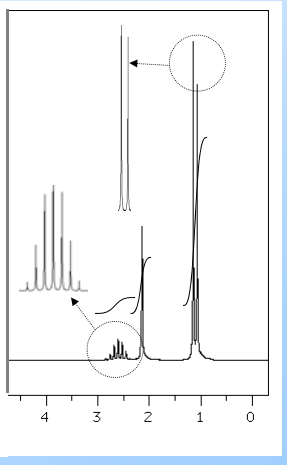
Which isomer of $C_5H_{10}O$ gives the following $^1$H NMR spectrum?



# $^{13}$C NMR SPECTROMETRY

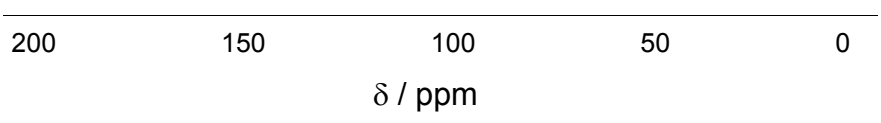
## Introduction

$^{13}$C (*not* $^{12}$C) has nuclear spin

However, $^{13}$C is only present at 1.1% abundance

- Signals are weak
- Spectra usually acquired without multiplicity information

- Larger range of chemical shifts (0 to >200 ppm)



## Types of Information available from a $^{13}C$ NMR spectrum

A $^{13}C$ nuclear magnetic resonance spectrum contains information about the:

(a) number of different types of carbon

- Each peak corresponds to a different *type* of carbon

(b) type of carbons and proximity to functional groups

- Chemical shift provides information about the type of carbon present

Unlike $^{1}H$ NMR spectra, simple $^{13}C$ NMR spectra *do not* provide information about the:

relative number of each type of proton

or

number of adjacent protons or carbons

---

# USING DATA TO DETERMINE STRUCTURE

1. Write down conclusions from *each individual technique*
   - Use combustion analysis to determine empirical formula, and mass spectrometry to give molecular weight (and molecular formula)
   - Calculate number of rings and double bonds from molecular formula (SODAR)
   - Determine presence of functional groups present from infrared spectroscopy.
   - Use $^{1}H$ and $^{13}C$ NMR spectroscopy to identify other structural features.
2. Use these conclusions to determine the structure
3. *Check your answer* (predict the spectra; do your predicted spectra match the data provided?)

# USING SPECTRAL INFORMATION AND OTHER DATA TO DETERMINE THE STRUCTURE OF AN UNKNOWN COMPOUND

Elemental Analysis: C, 54.51; H, 9.09

Mass spectrometry: *m/e* M+, 88

**A. If you are provided with the elemental analysis (mass% C,H,O...), determine the *empirical* formula**

i.e., ratio of atoms, C : H : O : ... = mass% C/12 : mass %H/1 : mass% O/16 : ...

empirical formula:_____

**REMEMBER: The molecular formula might be an integral times the empirical formula**

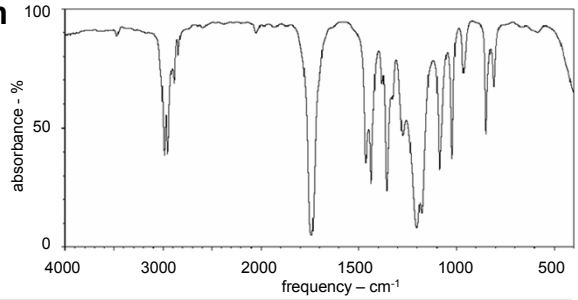
**If you are provided with the molecular weight (from mass spectrometry), determine the *molecular formula***

empirical formula weight =_____ molecular weight = _____ molecular formula:_____

**Determine the number of sites of unsaturation (i.e., SODAR = π bonds + rings):**

SODAR = (2#C + 2 - #H - #Hal + #N) / 2 ; SODAR=_____

## Infrared Spectrum




B. Bonds vibrate at certain frequencies. Determine the bonds present (and hence the functional groups) by considering the infrared spectrum

**i.** *Does your compound contain oxygen* Y ? N *If there is no oxygen, go to part Bii.*

**(a)** C=O bonds vibrate at approximately 1700 $cm^{-1}$, usually giving rise to a strong absorption. *Is there a strong absorption around 1700 $cm^{-1}$?* Some tables list frequencies for specific carbonyl-containing functional groups.

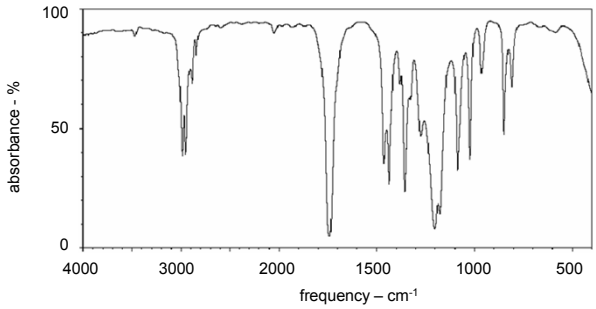
Y ? N Conclusion:_____

**(b)** C-O bonds vibrate at approximately 1200-1000 $cm^{-1}$; these peaks are usually strong. *Is there a strong absorption at 1000-1200 $cm^{-1}$?*

Y ? N Conclusion:_____

**(c)** O-H bonds give rise to a broad vibration band; in alcohols this appears at approximately 3300 $cm^{-1}$, but in carboxylic acids this band is very broad and might also appear between 2800 and 3200 $cm^{-1}$ (which overlaps with sharp C-H bond vibrational bands). If nitrogen is present, remember that N-H bonds also vibrate at 3000-3500 $cm^{-1}$. *Is there a broad absorption in the 3500-3000 $cm^{-1}$ range?*

Y ? N Conclusion:_____




**(d)** Based on the presence or absence of vibrational bands arising from *covalent bonds* to oxygen, you should be able to predict the *functional groups* present in the molecule. Circle the combination of bonds present and the corresponding functional group:

| *Bonds Present* | *Absent* | *Functional Group* | *BondsPresent* | *Absent* | *Functional Group* |
|---|---|---|---|---|---|
| C=O, O-H, C-O | - | acid | C-O | C=O, O-H | ether |
| C=O, C-O | O-H | ester | C=O | O-H, C-O | aldehyde or ketone |
| O-H, C-O | C=O | alcohol | C=O, N-H | O-H, C-O | 1° or 2° amide |

**ii.** Other common vibration bands to look for are those for C≡C and C=C. If nitrogen is present, look for C□N and N-H vibration bands. *Are any of these bands present?*

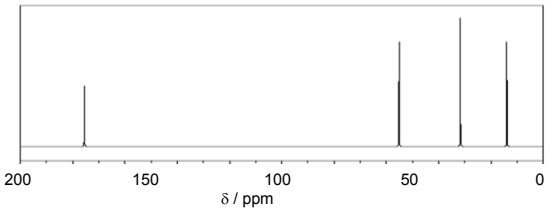
Y ? N Conclusion:_____

**iii.** $sp^2$ C-H bonds (in arenes and alkenes) give rise to a *sharp* vibrational band at 3100-3000 $cm^{-1}$. *Is there a sharp absorption at 3100-3000 cm-1?*

Y ? N Conclusion:_____

**iv**. *Draw the functional groups indicated by the infrared spectrum (i.e., structures from i(d) , ii and iii)*

## $^{13}C$ NMR Spectrum




**C. Consider the $^{13}C$ NMR spectrum...**

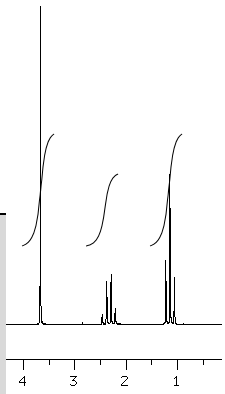
**i.** Each type of carbon gives rise to a separate singlet *How many types are carbon are there?*

_____

**ii.** *The $^{13}C$ chemical shift gives you a clue about the type of carbon (i.e., carbonyl, aromatic, alkenes) and the presence of electronegative substituents.*

Conclusion:_____

# $^1$H NMR Spectrum




**D. Certain common features give rise to recognizable patterns in the $^1$H NMR spectrum...**

**i.** Ethyl groups always give rise to a quartet (2H) downfield from a triplet (3H). *Is there a quartet downfield from a triplet?*

Y N Conclusion:_____

**ii.** *iso*-Propyl groups always give a septet (1H) downfield from a doublet (6H). Remember, you might not see the weak outside peaks in the septet. *Is there a septet downfield from a doublet?*

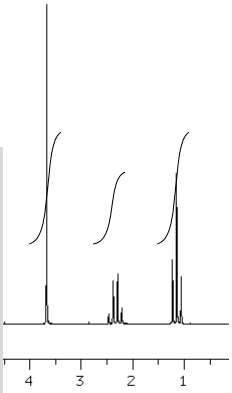
Y N Conclusion:_____

**iii.** *tert*-Butyl groups always give a singlet (9H) at ca. $\delta$1.2. *Is there a singlet at ca. $\delta$1.2?*

Y N Conclusion:_____

**iv.** *If there are ethyl or isopropyl groups: consider the chemical shift of the downfield signal, it gives you a clue about the substituent (i.e., "X" in $CH_3CH_2$-X or $(CH_3)_2CH$-X).*

Conclusion:_____




**v.** Aromatic protons appear at $\delta$6.5-8.5. *Is there a signal at $\delta$6.5-8.5?*

Y N Conclusion:_____

**vi.** *If there are aromatic protons: consider the multiplicity and integration, they give you clues about the substitution pattern?*

Conclusion:_____

**vii.** Certain functional groups that you have already identified by infrared give rise to specific signals in the $^1$H NMR, such as acid (-$CO_2$**H**), aldehyde (-C**H**O), alcohol (-O**H**), amine (-N**H**). *Do signals corresponding to these functional groups appear in the $^1$H NMR spectrum?*

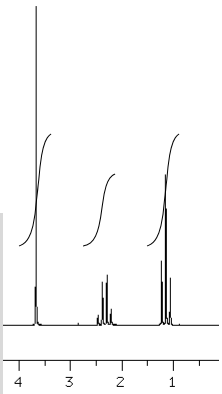
Y N Conclusion:_____

**viii.** Are there any other singlets or multiplets which you have not assigned? If so, consider the multiplicity and integration. Here is a list of common isolated structural features (i.e., without neighboring protons) and their corresponding signals (multiplicity and integration). *Do any of these appear in the spectrum? (Circle the combination of peaks and the structural subunit).* You will also have to consider vinylic protons in D(x).

| | | | | |
|---|---|---|---|---|
| C**H**-C**H** | d(1) d(1) | C$H_2$-C$H_2$ | t(2) t(2) | C**H**-C$H_3$ q(1) d(3) |
| C**H**-C$H_2$ | t(1) d(2) | C$H_3$ | s(3) | |

**ix.** If you have identified additional fragments in part viii: consider the chemical shift of the downfield signal, it gives you a clue about substituents.

Conclusion:_____




**ix.** *If any of these multiplets appear: consider the chemical shift of the downfield signal, it gives you a clue about the substituents on the fragment (Remember that substitutent effects are cumulative).*

Conclusion:_____

**x.** Vinylic protons appear at δ4.5-6.5. *Are there signals at δ4.5-6.5 which you have not yet accounted for?*

Y N Conclusion:_____

**xi.** *If there are vinylic protons: consider the multiplicity and integration, they give you clues about the substitution pattern.*

Conclusion:_____

**xii.** *Draw the substructures derived from the appearance of the $^1$H NMR spectrum (i-xi).*

## Bringing it all together

**E. If you are provided with the molecular formula: do you need to account for any other atoms in the molecule other than those determined in parts B,C and D?**

Y N Remaining atoms:_____

**F. ...Bring it all together**

*Draw the functional groups derived from IR (B), substructures derived from NMR (C and D), and any other atoms left over in the molecular formula (E).*

***G. FINAL STRUCTURE***

*Combine these fragments in such a way that the valency of each atom (H=1, C= 4, O=2, N=3) and the number of sites of unsaturation, and formula are satisfied. Remember to consider symmetrical structures.*

***Check your answer: predict the spectra of your final structure, it should be the same as those provided***

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**Types of Questions**

- Use data from elemental analysis, infrared spectroscopy and nuclear magnetic resonance spectrometry ($^{1}H$ and $^{13}C$) to determine the structure of organic compounds.