Tool Box

* Databooklet Table 26

Bond	Organic molecules	Wavenumber (cm^{-1})	Intensity
C–I	iodoalkanes	490–620	strong
C–Br	bromoalkanes	500–600	strong
C–Cl	chloroalkanes	600–800	strong
C–F	fluoroalkanes	1000–1400	strong
C–O	alcohols, esters, ethers	1050–1410	strong
C=C	alkenes	1620–1680	medium-weak; multiple bands
C=O	aldehydes, ketones, carboxylic acids and esters	1700–1750	strong
C≡C	alkynes	2100–2260	variable
O–H	carboxylic acids (with hydrogen bonding)	2500–3000	strong, very broad
C–H	alkanes, alkenes, arenes	2850–3090	strong
O–H	alcohols and phenols (with hydrogen bonding)	3200–3600	strong, broad
N–H	primary amines	3300–3500	medium, two bands

Figure 1: Infra-red Data

* $O_2 \rightarrow O \cdot + O \cdot$
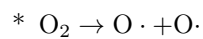
* $c = \lambda \cdot f$

* Fingerprint region: wave number ranges under $1500 cm^{-1}$

* IUPAC Naming of organic molecules...

1 Infra-red Spectroscopy (IR)

Learning Objectives

- Understand that infra-red (IR) spectroscopy can be used to identify functional groups

- Interpret a simple IR spectrum

- Link each of the main peaks in an IR spectrum to their correct functional group

- Distinguish between two compounds based on their infrared spectra

1.1 Background Information

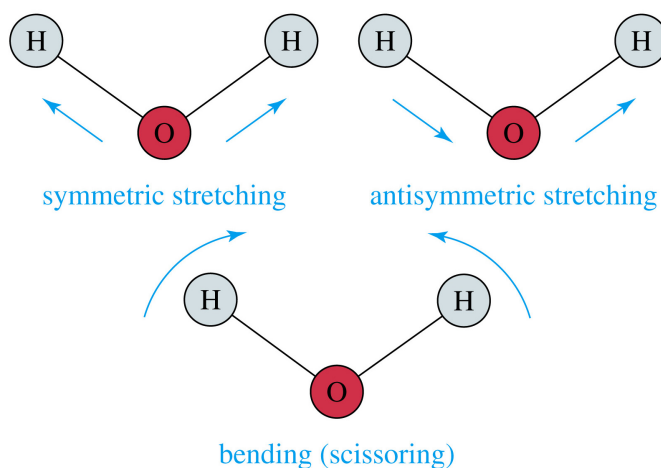Bonds <u>oscillate</u>, adding energy increases **amplitude** of oscillating.

Figure 2: Stretchings and Bending

1. Symmetric stretch

2. Asymmetric stretch

3. Symmetric bend

1.2 Frequencies of Chemical Bond

1. **Bond Strength**
   Multiple Bonds ¿ Single Bond
   Hence the frequencies of multiple bonds are **higher** than single bond

2. **Relative Atomic Mass**
   Bigger Atomic Mass $\rightarrow$ Higher Frequencies

1.3 Introduction to Wavenumber

Wavenumber $= \frac{1}{\lambda}$

Unit: cm^{-1}
* For convenience to calculate

1.4 Methods to Interpret Wavenumber vs Abundance Graph

A step by step guide (sort of)

1. Identify the peaks (and their wavenumber), and refer to data booklet table 26 for the functional groups.

2. If there is a **broad peak** at just below 3400 (in 2500 - 3300) cm^{-1}, then there is presence of hydrogen bonding due to the hydroxyl (OH) group. Combined with a peak in 1700 (C-O), it becomes carboxylic acid.

3. Do note that

2 ^{1}H-NMR Spectroscopy

HNMR: Proton Nuclear Magnetic Resonance
Nuclear magnetic resonance (NMR) spectroscopy identifies the structure of the molecule.

It reflects the **radiowaves** part of Electromagnetic Waves.

Learning Objectives

- Understand what is meant by TMS in HNMR spectroscopy

- Interpret a simple HNMR spectroscopy

- Link each of the maximum peaks in an HNMR spectroscopy to their correct hydrogen environment

- Distinguish between two compounds based on their HNMR spectroscopy

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2.1 Hydrogen Environment, TMS, and Chemical Shifts

Step by Step Process:

1. The hydrogen nuclei in different chemical environments produce different signals in the spectrum.

2. Standard signal emitted by TMS, which is called **tetramethylsilane**, having 12 Hydrogen atoms. Its value is 0 ppm.
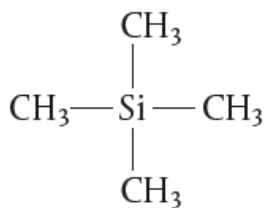
Figure 3: Structure of TMS

3. The position of NMR signals relative to the standard signal is the chemical shifts of the proton.

2.2 Interpret a [1] H-NMR Spectrum

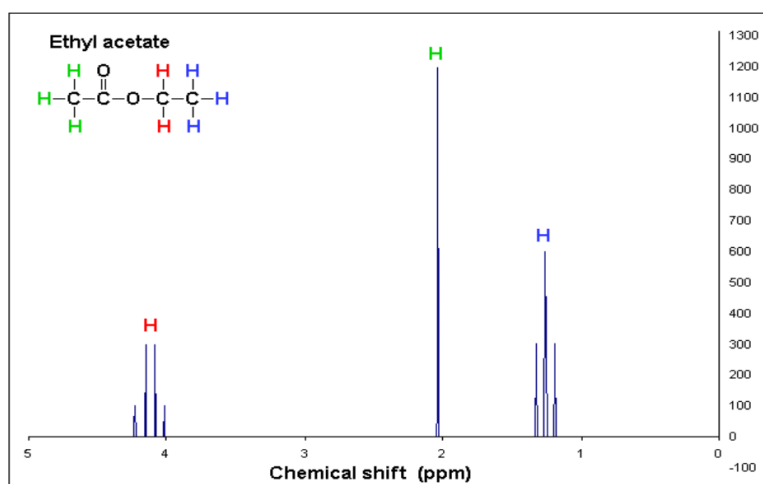To help with better understanding, an example of HNMR spectrum is used in this guide.

Figure 4: HNMR Spectrum of Ethyl Acetate

2.2.1 Identify the Chemical Environment from the Peaks

Step by Step Process:

1. Find how many peaks do the element have on the spectrum. (Usually it's H)

2. Then the number of peaks correspond to the number of chemical environments.

3. Notice that some hydrogen atoms might have the same chemical environment because it depends on the atoms/groups it could "see" (it directly connected to within the connected carbon)

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2.2.2 Interpret Chemical Shifts

Step by Step Process:

1. The value of chemical shifts is unique according to different chemical environments.

2. Find the value in ppm to match with Data Booklet Table 27

3. Find the type of protons (functional group) of that organic compound.
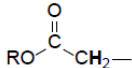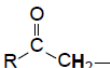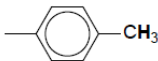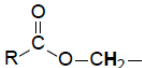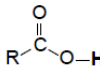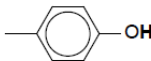
Type of proton	Chemical shift (ppm)
—CH$_3$	0.9–1.0
—CH$_2$R	1.3–1.4
—CHR$_2$	1.5
RO—C(=O)—CH$_2$—	2.0–2.5
R—C(=O)—CH$_2$—	2.2–2.7
phenyl—CH$_3$	2.5–3.5
—C≡C—H	1.8–3.1
—CH$_2$-Hal	3.5–4.4
R—O—CH$_2$—	3.3–3.7
R—C(=O)—O—CH$_2$—	3.7–4.8
R—C(=O)—O—H	9.0–13.0
R—O—H	1.0–6.0
—CH=CH$_2$	4.5–6.0
phenyl—OH	4.0–12.0

Figure 5: HNMR Chemical Shifts Data

2.2.3 Interpret the Area Under Graph

Step by Step Process:

1. Find the ratio of the absorption values of different hydrogen peaks.

2. Then the ratio is between the number of protons (hydrogens) of different environments sending the signals.

3. The number of hydrogens is determined.

3   Mass Spectroscopy (MS)

3.1   How Mass Spectroscopy Works?

1. Mass spectrometry (MS) identifies the relative atomic mass and molecular mass.

2. The scientists use an electron to knock another electron from the compound to make cations.
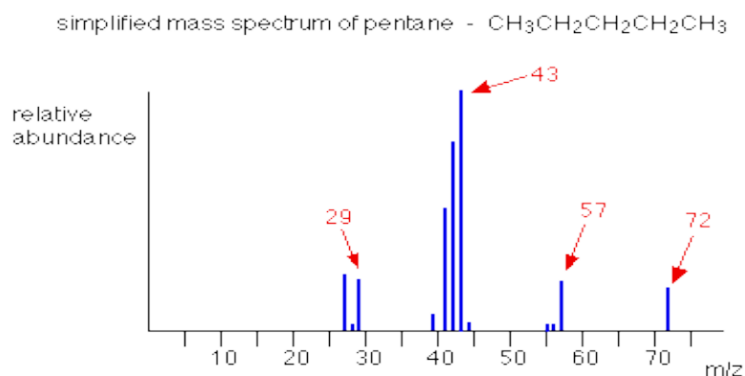
3.2   How to identify the compound from MS?

Figure 6: Mass Spectrometry of Pentane

1. Add Method: To evaluate the number originally appeared. (Such as 29, may corresponding to a CH_3CH_2 group)

2. Subtract Method: To subtract the smaller number from the bigger one. (72-57=15, corresponding to a CH_3 group)

4   Index of Hydrogen Deficiency (IHD)

It reflects the degree of Unsaturation. (Multiple bonds $\rightarrow$ unsaturated)

1. For a C——H (single bond), IHD = 0
2. For a C===H (double bond), IHD = 1
3. For a C≡≡≡H (triple bond), IHD = 2

The general formula is:

$$IHD = \frac{1}{2} \cdot (2 \cdot carbon + 2 - hydrogen + halogen - nitrogen)$$