MSJChem

Tutorials for IB Chemistry

Topic 11 Measurement and data processing SL

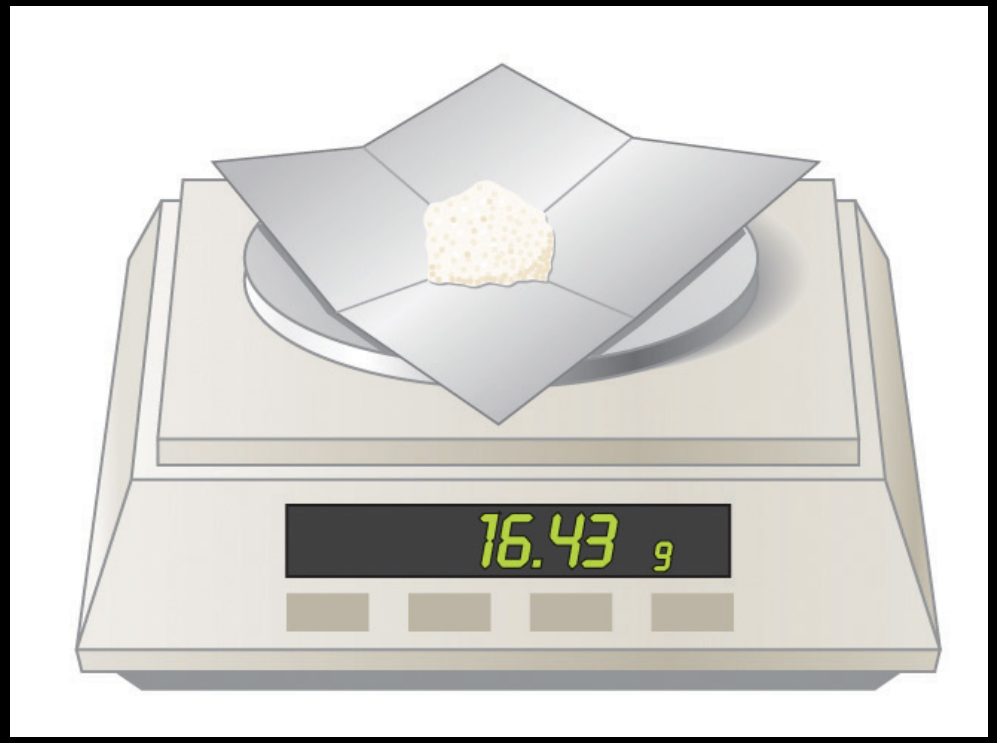
MSJChem

Tutorials for IB Chemistry

Absolute and percentage uncertainties

Digital apparatus

The absolute uncertainty of digital apparatus is ± the smallest scale division.



Absolute uncertainty of mass balance is ± 0.01 g

Mass of $CaCO_3$ = 16.43 ± 0.01 g

Percentage uncertainty:

$$\frac{0.01}{16.43} \times 100 = 0.06\ \%$$

Digital apparatus

Absolute uncertainty of mass balance is ± 0.0001 g

Mass of empty beaker = 149.2101 ± 0.0001 g

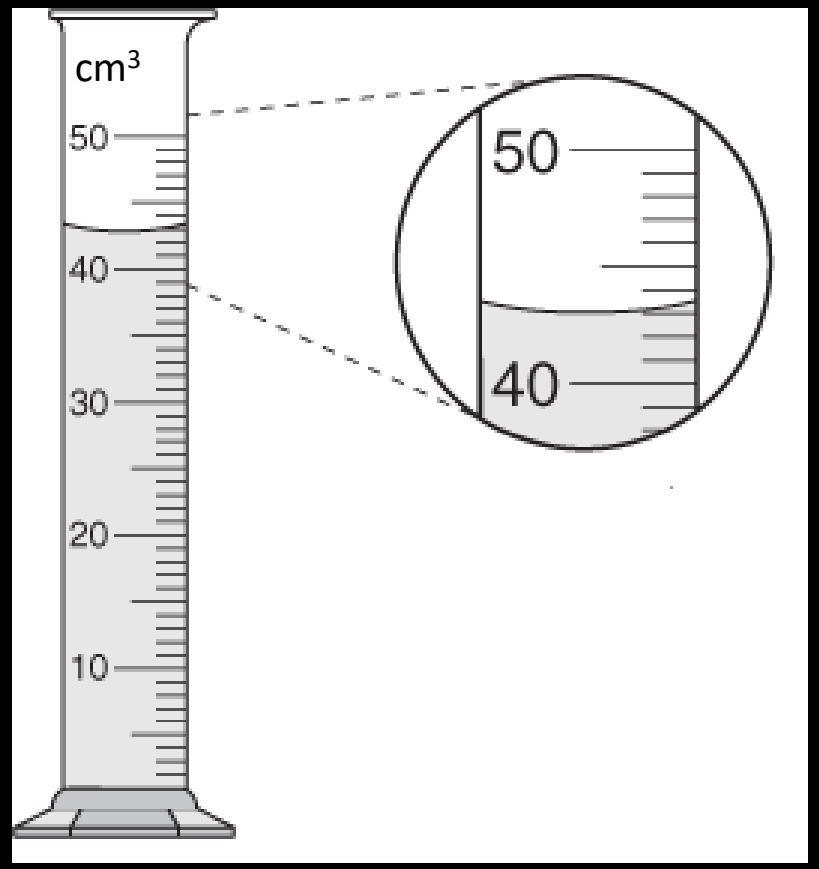
Percentage uncertainty:

$$\frac{0.0001}{149.2101} \times 100 = 7 \times 10^{-5}\ \%$$

MSJChem
Tutorials for IB Chemistry

Analog apparatus

The absolute uncertainty of analog apparatus is ± half the smallest scale division.



Absolute uncertainty of measuring cylinder is ± 0.5 cm^3

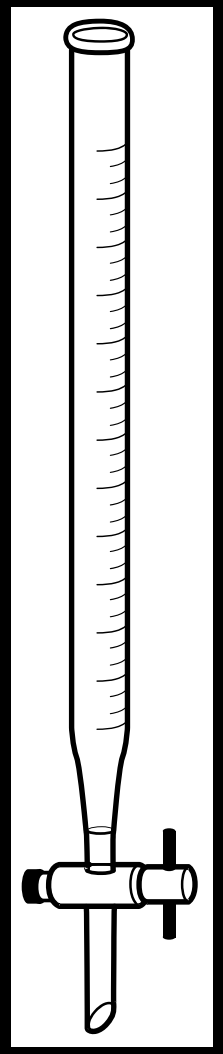
Volume of H_2O = 43.0 ± 0.5 cm^3

Percentage uncertainty:

$$\frac{0.5}{43.0} \times 100 = 1\%$$

MSJChem
Tutorials for IB Chemistry

Analog apparatus



A burette measures to two decimal places with the last digit being a 0 or 5.

The absolute uncertainty of a burette is ± 0.05 cm^3

	Trial 1	Trial 2	Trial 3	Trial 4
Initial volume of $NaOH_{(aq)}$ (± 0.05 cm^3)	0.00	0.00	0.00	0.00
Final volume of $NaOH_{(aq)}$ (± 0.05 cm^3)	11.10	11.00	10.85	10.90
Total volume of $NaOH_{(aq)}$ (± 0.10 cm^3)	11.10	11.00	10.85	10.90
Colour change with phenolphthalein	dark pink	pink	light pink	light pink

Volume of $NaOH_{(aq)}$ = (10.85 + 10.90) ÷ 2 = 10.88 ± 0.10 cm^3

Percentage uncertainty: $\frac{0.10}{10.88} \times 100 = 0.9\%$

MSJChem

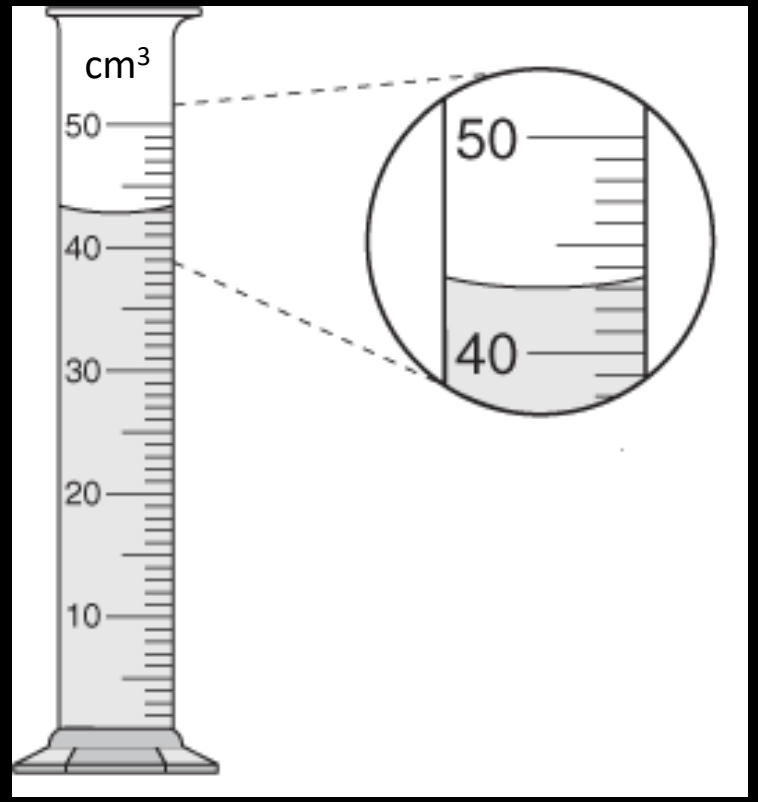
Tutorials for IB Chemistry

Quantitative and qualitative data

MSJChem
Tutorials for IB Chemistry

Quantitative data

Quantitative data is data taken from measurements made in the laboratory and is associated with random errors.



Qualitative data

Qualitative data includes non-numerical data obtained from observations, not from measurements.

Recording data

A results table should include quantitative data with units and uncertainties.

Quantitative data should be recorded to the appropriate precision.

	Trial 1	Trial 2	Trial 3	Trial 4
Initial volume of $NaOH_{(aq)}$ ($\pm$ 0.05 cm^3)	0.00	0.00	0.00	0.00
Final volume of $NaOH_{(aq)}$ ($\pm$ 0.05 cm^3)	11.10	11.00	10.85	10.90
Total volume of $NaOH_{(aq)}$ ($\pm$ 0.10 cm^3)	11.10	11.00	10.85	10.90
Colour change with phenolphthalein	dark pink	pink	light pink	light pink

Qualitative data should also be recorded.

MSJChem

Tutorials for IB Chemistry

Random and systematic errors

Random errors

Random errors are caused by unpredictable changes in the experiment (in the conditions or apparatus). With random errors, there is an equal probability of the measured value being too high or too low.

Examples of random error:

- Changes in the environment during the experiment (such as a change in the room temperature).
- Observer misinterpreting the reading.
- Insufficient data (not conducting repeat trials).

Random errors

Random errors cannot be eliminated but can be reduced by conducting repeat trials.
They can also be reduced by using precise apparatus (such as using a volumetric pipette rather than a beaker to measure volume).

Uncertainty of a 50 cm^3 beaker = ± 5 cm^3

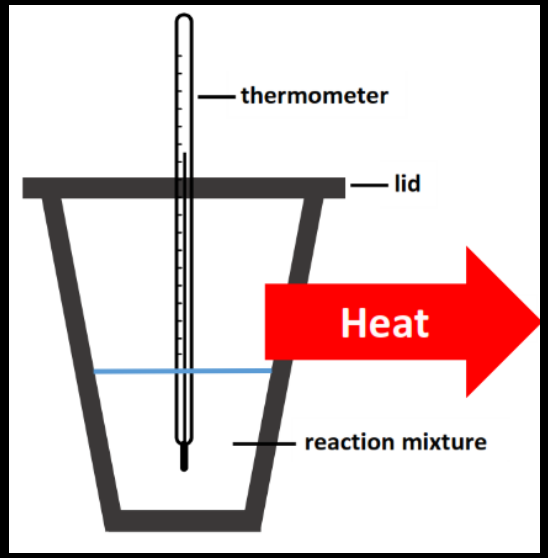
Uncertainty of a 20 cm^3 volumetric pipette = ± 0.08 cm^3

Systematic errors

Systematic errors occur as a result of a flaw in the experimental design or apparatus.

Systematic errors cause the measured values to be consistently higher or lower than the actual value.

They cannot be reduced by conducting repeat trials.



Systematic errors

Examples of systematic errors:

- Heat loss in an experiment to measure enthalpy change.
- Losing a product (such as a gas) in a reaction.
- Overshooting the endpoint in a titration.
- Reading from the top of the meniscus when measuring volume.
- Forgetting to zero a mass balance.

MSJChem

Tutorials for IB Chemistry

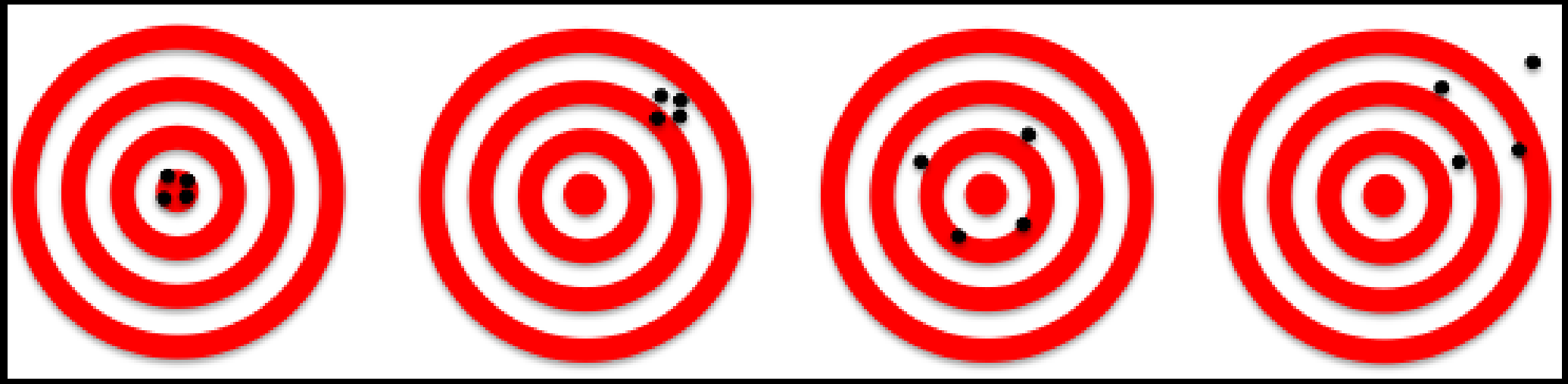
Accuracy and precision

MSJChem
Tutorials for IB Chemistry

Accuracy and precision

Accuracy refers to the closeness of a value to the true or actual value.

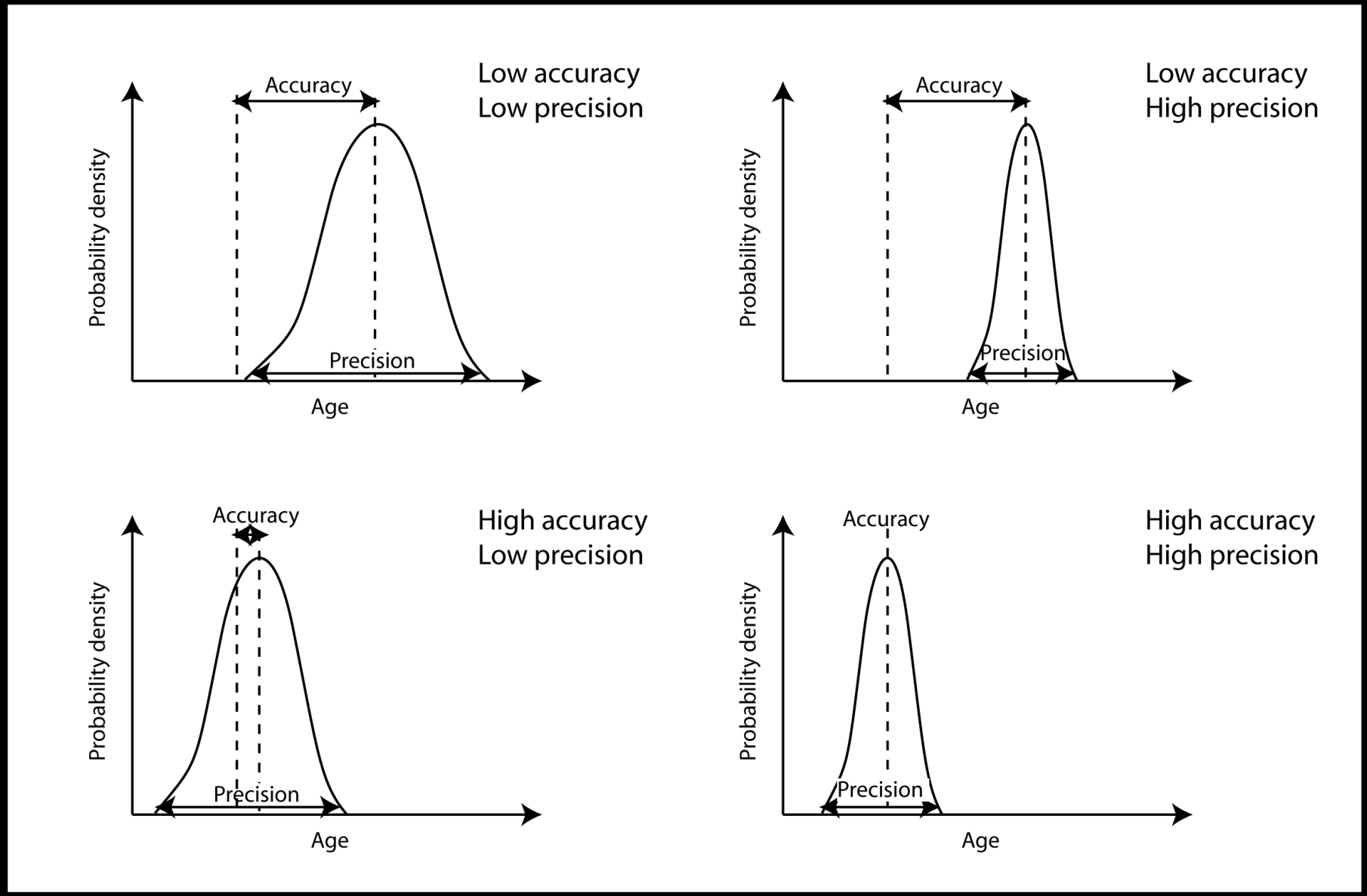
Precision refers to the closeness of a set of values to each other.



High accuracy High precision	High precision Low accuracy	Hugh accuracy Low precision	Low accuracy Low precision

MSJChem
Tutorials for IB Chemistry

Accuracy and precision

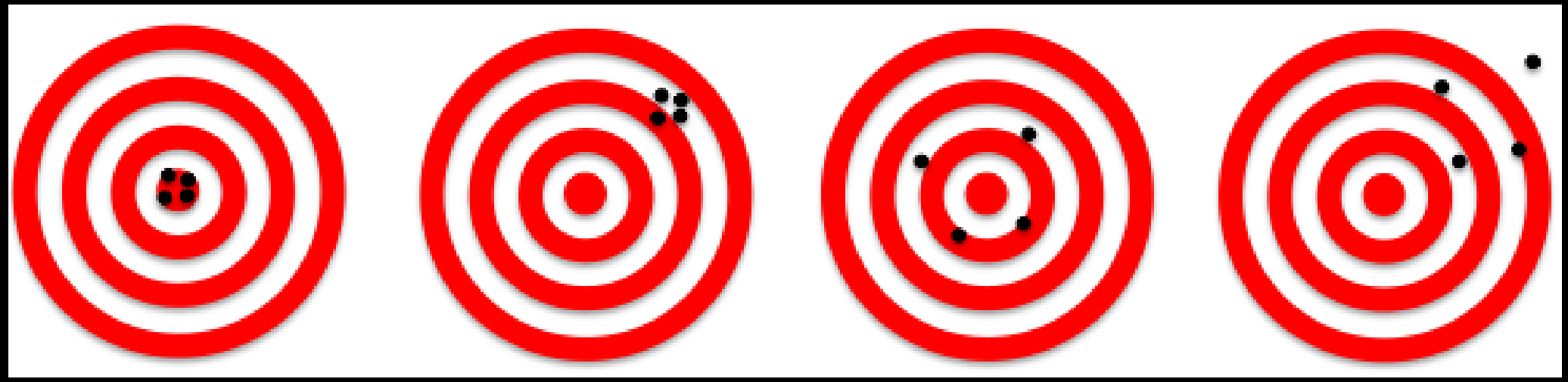


MSJChem
Tutorials for IB Chemistry

Accuracy and precision

Accuracy refers to the closeness of a value to the true or actual value.

Precision refers to the closeness of a set of values to each other.



Accurate and precise

Precise but not accurate

Accurate but not precise

Neither accurate nor precise

MSJChem

Tutorials for IB Chemistry

Propagation of uncertainties

Propagation of uncertainties

In an experiment to measure the enthalpy change of a reaction the following quantitative data was collected:

Volume of water in calorimeter = 50.0 ± 0.5 cm^3

Trial	Initial temperature of water (± 0.5 °C)	Maximum temperature of water (± 0.5°C)	Change in temperature of water (± 1.0°C)
1	18.5	26.0	6.5
2	18.5	25.5	7.0
3	18.5	26.5	8.0

Calculate average temperature: $\frac{(6.5+7.0+8.0)}{3} = 7.2°C$

Average change in temperature = 7.2 ± 1.0°C

Propagation of uncertainties

Calculate the heat (Q) released:

Density of water = 1 g cm^{-3}

Specific heat capacity of water = 4.18 J g^{-1} $^oC^{-1}$

$$Q = mc\Delta T$$

$$Q = 50.0 \times 4.18 \times 7.2 = 1504.8 \text{ J}$$

$$Q = 1.5 \times 10^3 \text{ J}$$

Propagation of uncertainties

Propagate uncertainties:

Uncertainty in temperature (already calculated) ± 1.0°C

Convert to percentage uncertainty: $\frac{1.0}{7.2} \times 100 = 14\ \%$

Uncertainty in volume of water ± 0.5 cm^3

Convert to percentage uncertainty: $\frac{0.5}{50.0} \times 100 = 1\%$

Add together percentage uncertainties: (1+14) = 15%

MSJChem
Tutorials for IB Chemistry

Propagation of uncertainties

$$Q = 1.5 \times 10^3 \text{ J} \pm 15\%$$

Convert back to absolute uncertainty: $\frac{15}{100} \times 1500 = 180$ J

$$Q = 1.5 \times 10^3 \pm 180 \text{ J}$$

MSJChem

Tutorials for IB Chemistry

Percentage error

MSJChem
Tutorials for IB Chemistry

Percentage error

Percentage error is a measure of how close the experimental value is to the theoretical or accepted value.

$$\% \text{ error} = \frac{(\text{experimental value}) - (\text{theoretical value})}{\text{theoretical value}} \times 100$$

If the experimental value is less than the theoretical value, the percentage error will be negative.
If it is greater than the theoretical value, the percentage error will be positive.

MSJChem
Tutorials for IB Chemistry

Percentage error

The experimental value for the enthalpy change of neutralization was found to be -49.6 $kJmol^{-1}$. The literature value for the enthalpy change of neutralization is -57.0 $kJmol^{-1}$. Calculate the percentage error.

$$\% \text{ error} = \frac{(-49.6)-(-57.0)}{-57.0} \times 100$$

$$\% \text{ error} = -13\%$$

A high percentage error indicates the presence of systematic errors (heat loss to the surroundings).

MSJChem

Tutorials for IB Chemistry

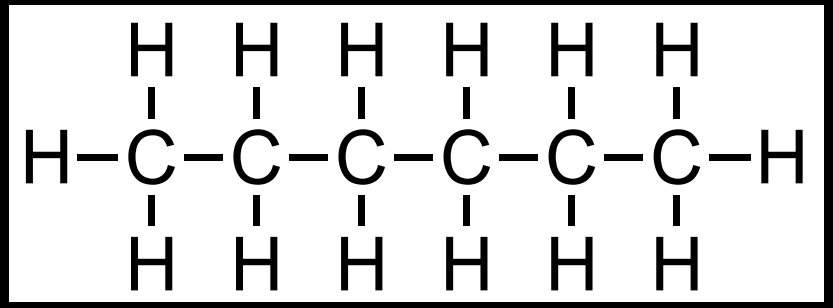
Index of hydrogen deficiency (IHD)

MSJChem
Tutorials for IB Chemistry

Index of hydrogen deficiency

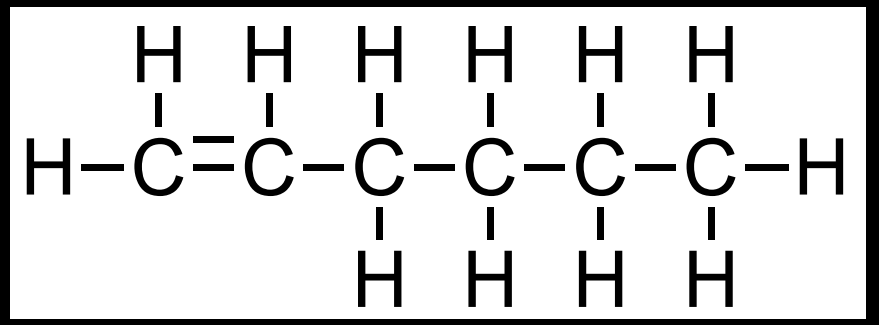
A saturated non-cyclic hydrocarbon has the maximum number of hydrogen atoms (C_nH_{2n+2})

hexane
C_6H_{14}



If any of the carbon to carbon single bonds are replaced by carbon to carbon double or triple bonds, or if the molecule contains a ring structure, there is a deficiency of hydrogen atoms.

hex-1-ene
C_6H_{12}



Index of hydrogen deficiency

The index of hydrogen deficiency (IHD) is a count of how many molecules of H_2 need to be added to convert the molecule to the corresponding saturated, non-cyclic molecule.

By calculating the IHD, we can tell from the molecular formula how many multiple bonds and rings are present in the molecule.

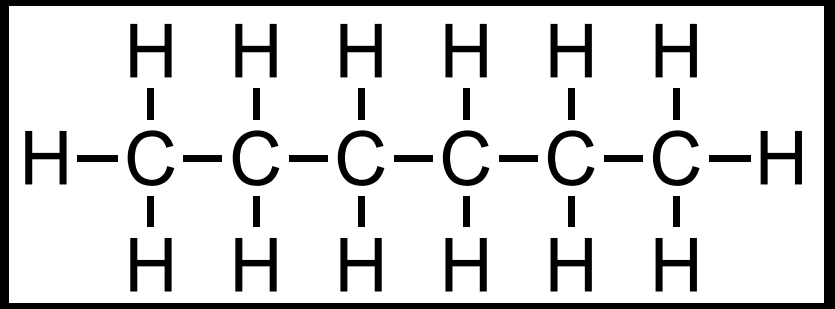
The IHD for a hydrocarbon with x carbon atoms and y hydrogen atoms is give by the equation:

$$\text{IHD} = \frac{(2x + 2 - y)}{2}$$

MSJChem
Tutorials for IB Chemistry

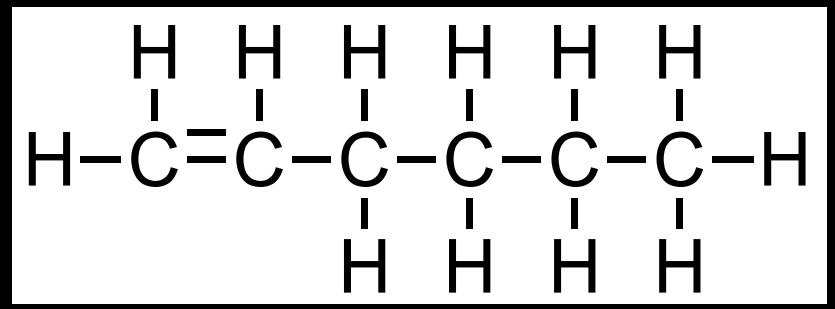
Index of hydrogen deficiency

hexane
C_6H_{14}



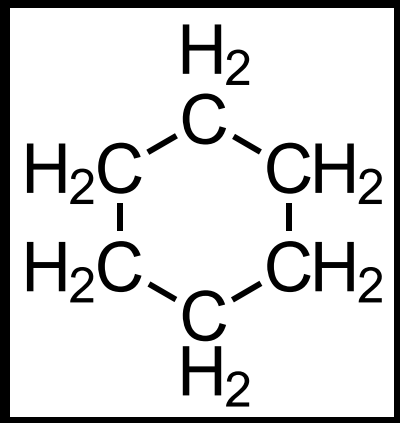
$$IHD = \frac{(12 + 2 - 14)}{2} = 0$$

hex-1-ene
C_6H_{12}



$$IHD = \frac{(12 + 2 - 12)}{2} = 1$$

cyclohexane
C_6H_{12}

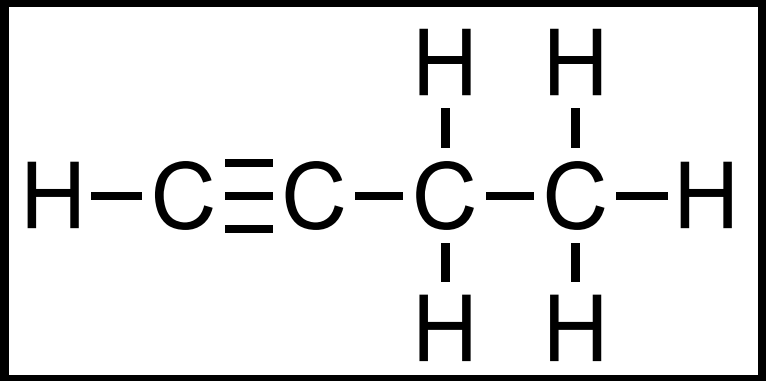


$$IHD = \frac{(12 + 2 - 12)}{2} = 1$$

MSJChem
Tutorials for IB Chemistry

Index of hydrogen deficiency

but-1-yne
C_4H_6



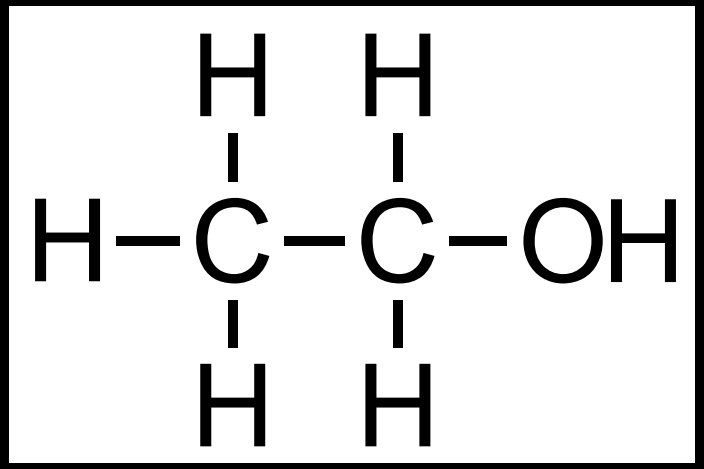
$$\text{IHD} = \frac{(8 + 2 - 6)}{2} = 2$$

Compounds that contain atoms other than hydrogen (H):

- sulfur (S) and oxygen (O) do not affect the IHD
- halogens (F, Cl, Br and I) are treated like H atoms
- nitrogen (N) – for each N atom, add one to the number of C atoms and H atoms

MSJChem
Tutorials for IB Chemistry

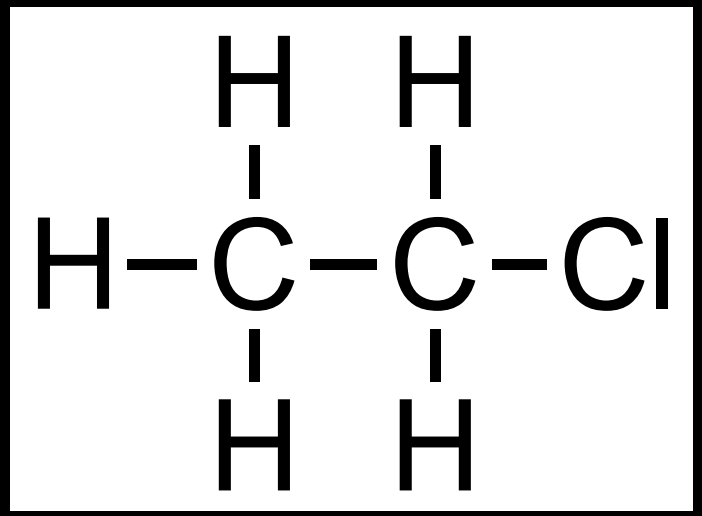
Index of hydrogen deficiency



ethanol

C_2H_5OH

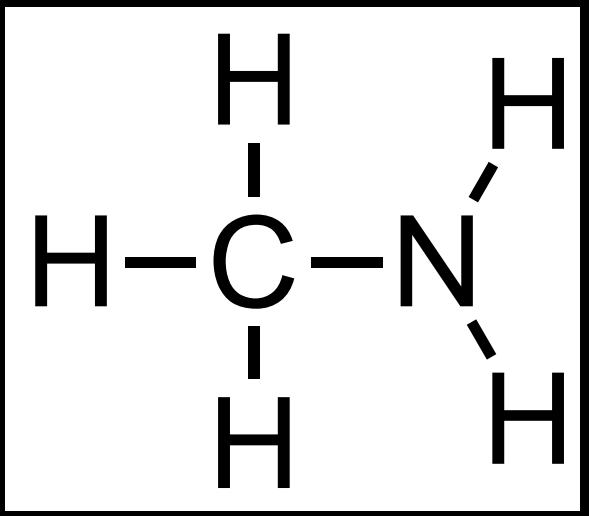
C_2H_6



chloroethane

C_2H_5Cl

C_2H_6



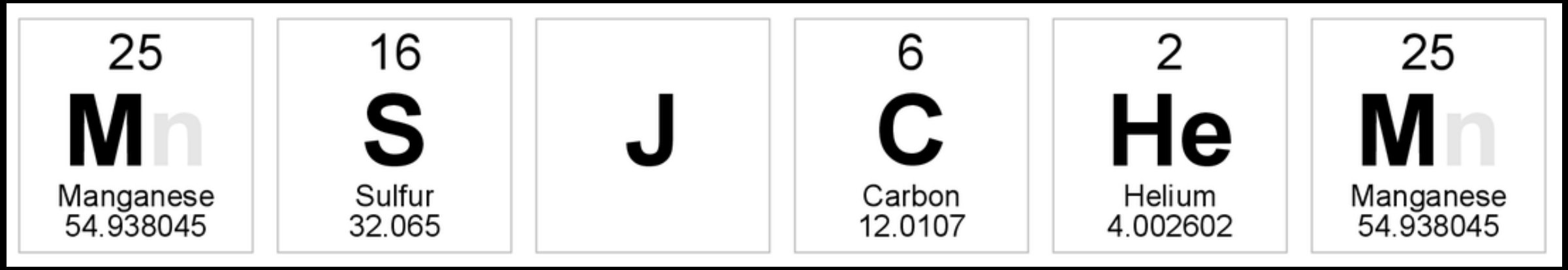
methylamine

CH_5N

C_2H_6

Index of hydrogen deficiency

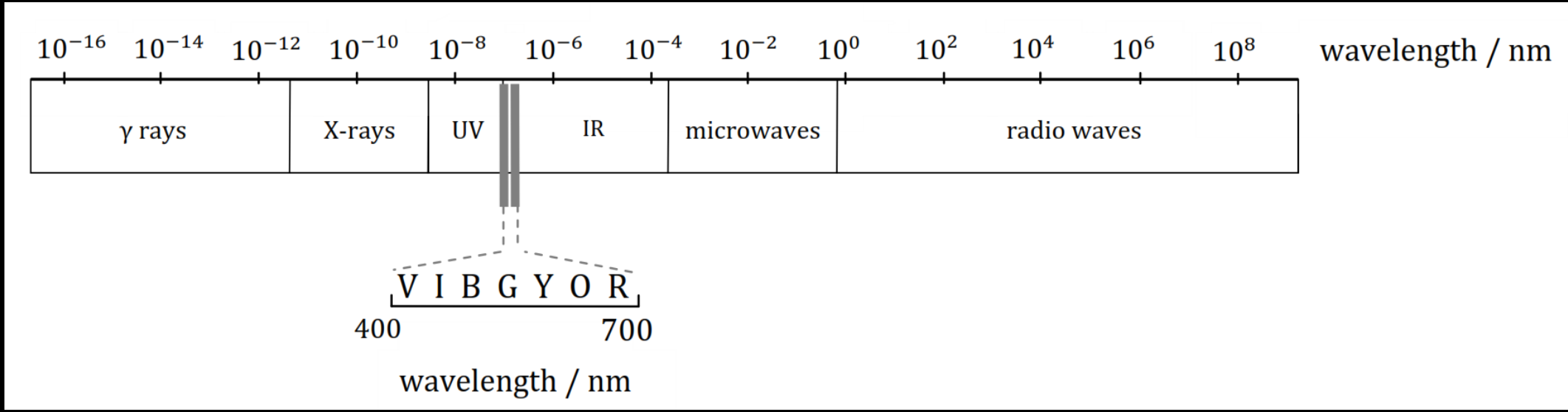
IHD	Multiple bonds/rings present in molecule	Example
0	single bonds (saturated, non-cyclic)	propane C_3H_8
1	double bond / ring structure	but-2-ene C_4H_8 cyclopropane C_5H_{10}
2	triple bond	propyne C_3H_4



Infrared spectroscopy

MSJChem
Tutorials for IB Chemistry

Infrared spectroscopy



When molecules absorb energy in the infrared region of the electromagnetic spectrum, it causes the bonds between the atoms to vibrate (the bonds stretch and bend).

The frequency of IR radiation that is absorbed is measured as the number of waves per centimeter (wavenumber cm^{-1})

MSJChem
Tutorials for IB Chemistry

Infrared spectroscopy

26. Infrared data

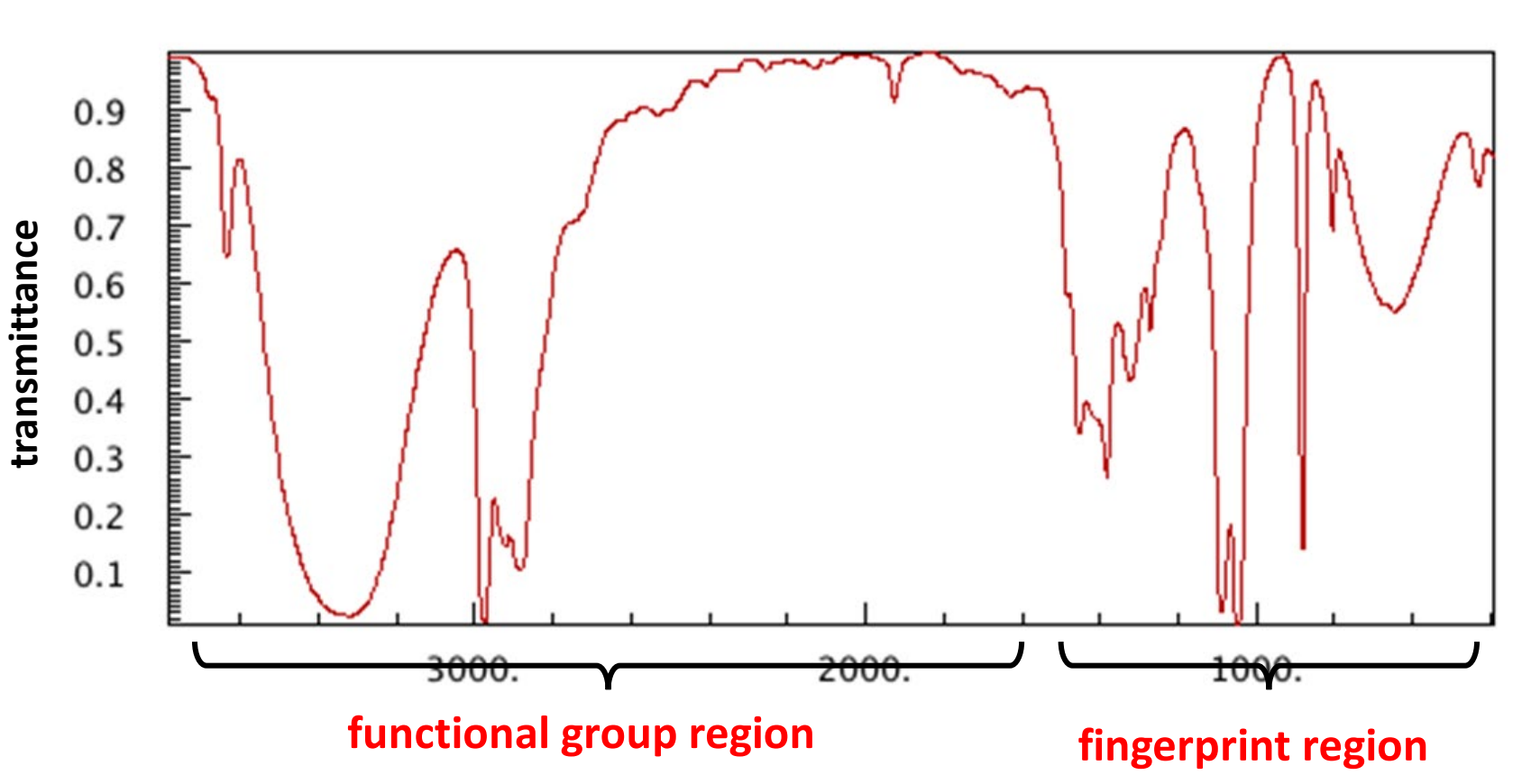
Characteristic ranges for infrared absorption due to stretching vibrations in organic molecules.

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	hydrogen bonding in carboxylic acids	2500–3000	strong, very broad
C–H	alkanes, alkenes, arenes	2850–3090	strong
O–H	hydrogen bonding in alcohols and phenols	3200–3600	strong, broad
N–H	primary amines	3300–3500	medium, two bands

MSJChem
Tutorials for IB Chemistry

Infrared spectroscopy

IR spectrum for ethanol C_2H_5OH



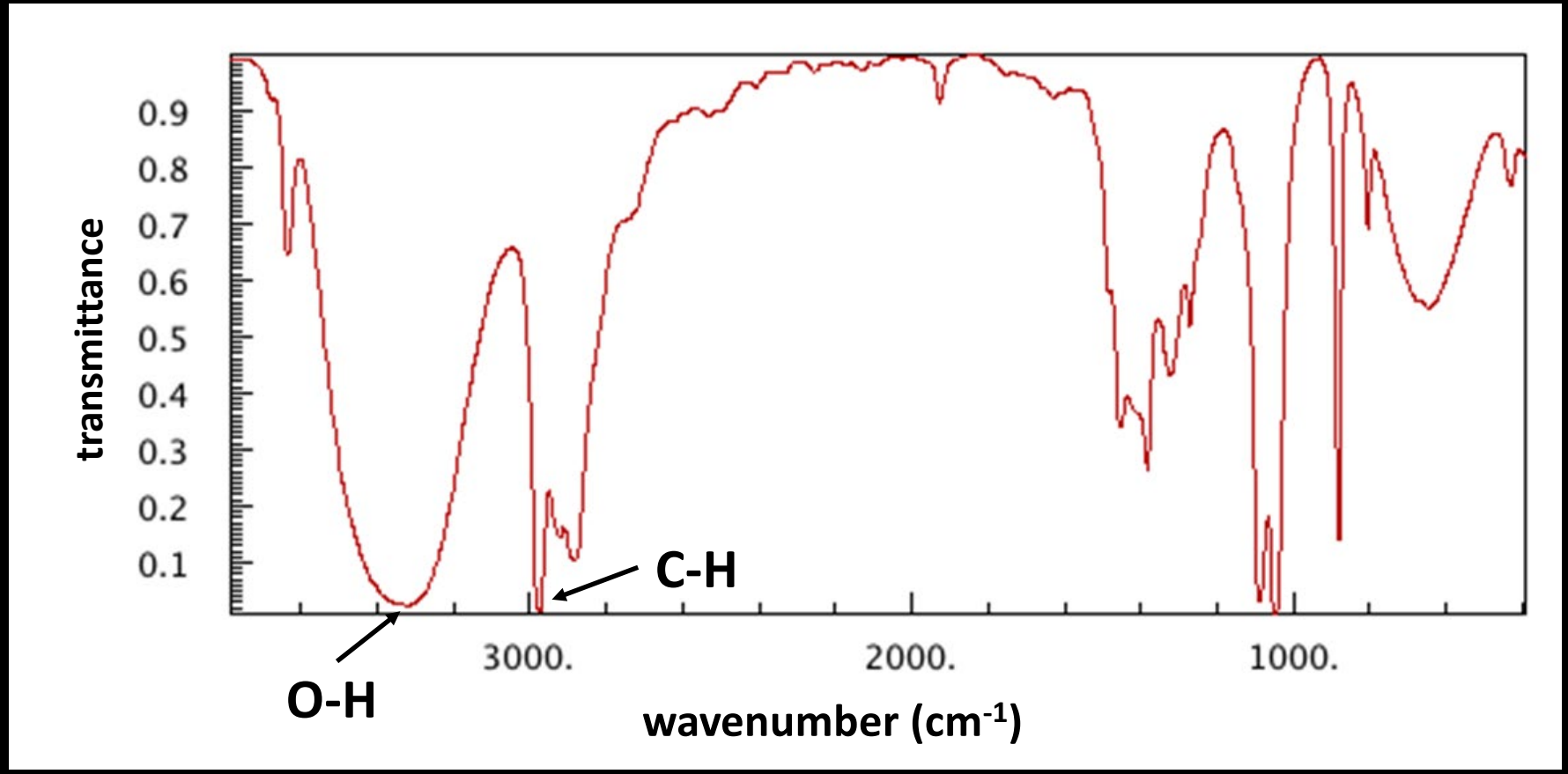
The region of an infrared spectrum in the range of about 500 to 1500 cm^{-1}
This region of the spectrum is almost unique for any given compound.

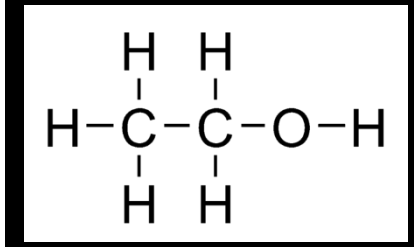
The fingerprint region can be used to identify an unknown compound by comparing with the IR spectra of known compounds.

MSJChem
Tutorials for IB Chemistry

Infrared spectroscopy

IR spectrum for ethanol C_2H_5OH



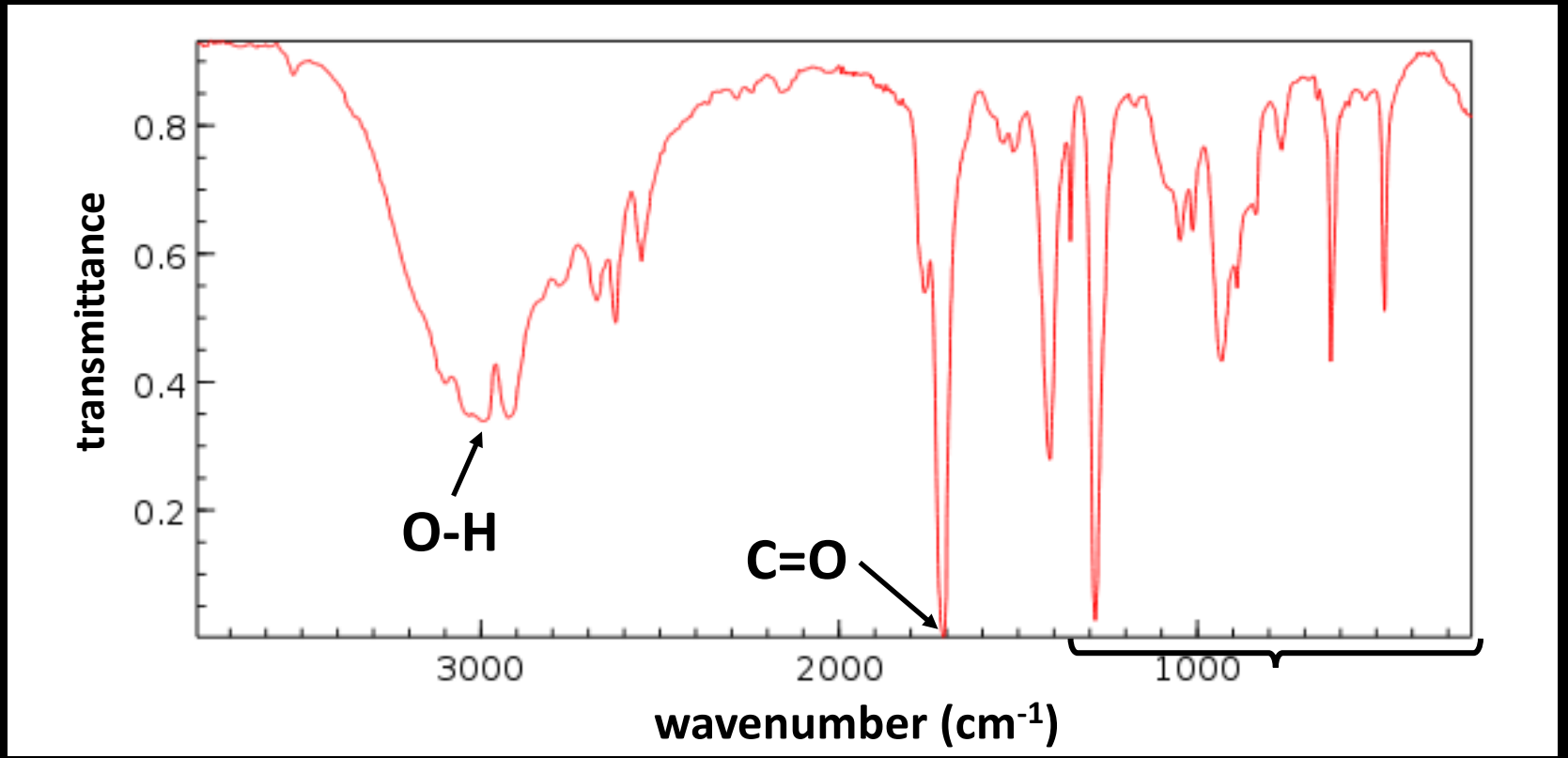


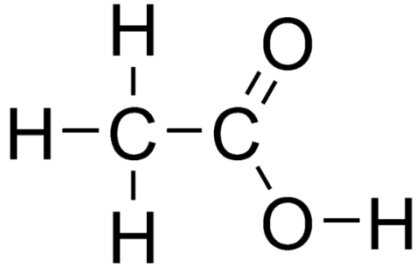
Bond	Organic molecule	Wavenumber (cm^{-1})	Intensity
C-H	alkanes, alkenes, arenes	2850 – 3090	strong
O-H	hydrogen bonding in alcohols and phenols	3200 – 3600	strong, broad

MSJChem
Tutorials for IB Chemistry

Infrared spectroscopy

IR spectrum for ethanoic acid CH_3COOH





Bond	Organic molecule	Wavenumber (cm^{-1})	Intensity
C=O	aldehydes, ketones, carboxylic acids and esters	1700 – 1750	strong
O-H	hydrogen bonding in carboxylic acids	2500 – 3000	strong, very broad

Infrared spectroscopy

A bond will only interact with IR radiation if it is a polar covalent bond (non-polar bonds do not absorb IR radiation).

Bond	Organic molecules	Wavenumber (cm^{-1})	Intensity
C–I	iodoalkanes	490–620	strong

The intensity of the band depends on the diploe moment of the bond:

- Strongly polar bonds produce strong bands
- Bonds with medium polarity produce medium bands
- Weakly polar bonds produce weak bands

MSJChem

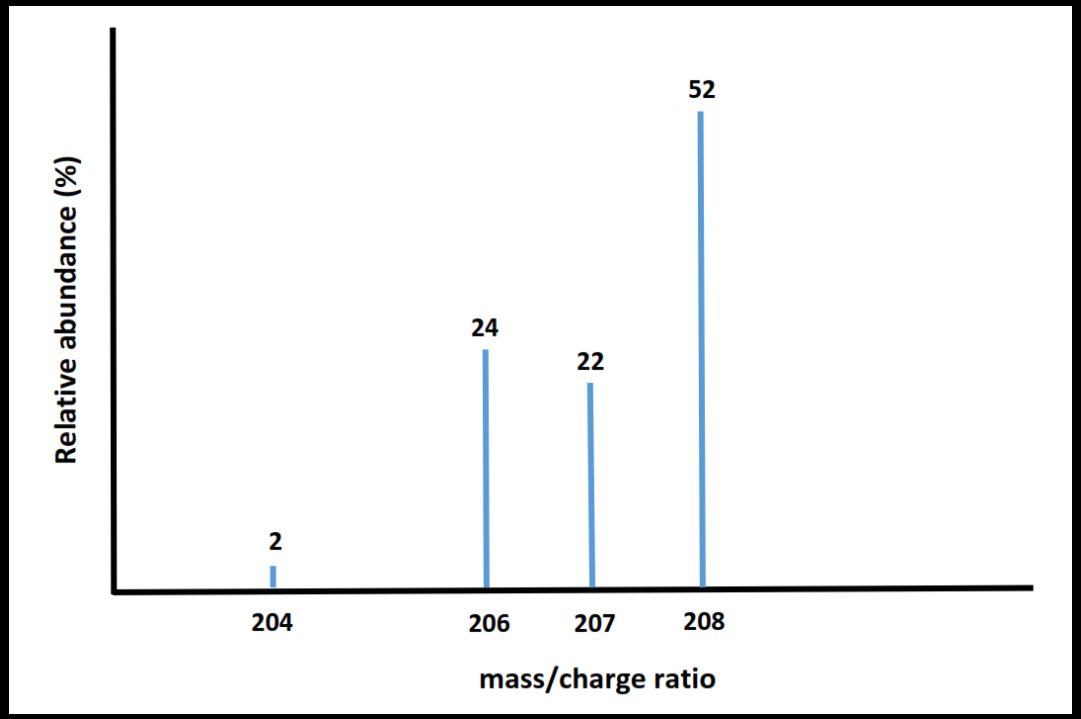
Tutorials for IB Chemistry

Mass spectrometry

MSJChem
Tutorials for IB Chemistry

Mass spectrometry

Mass spectrometry is used to determine the relative atomic mass (A_r) of an element.



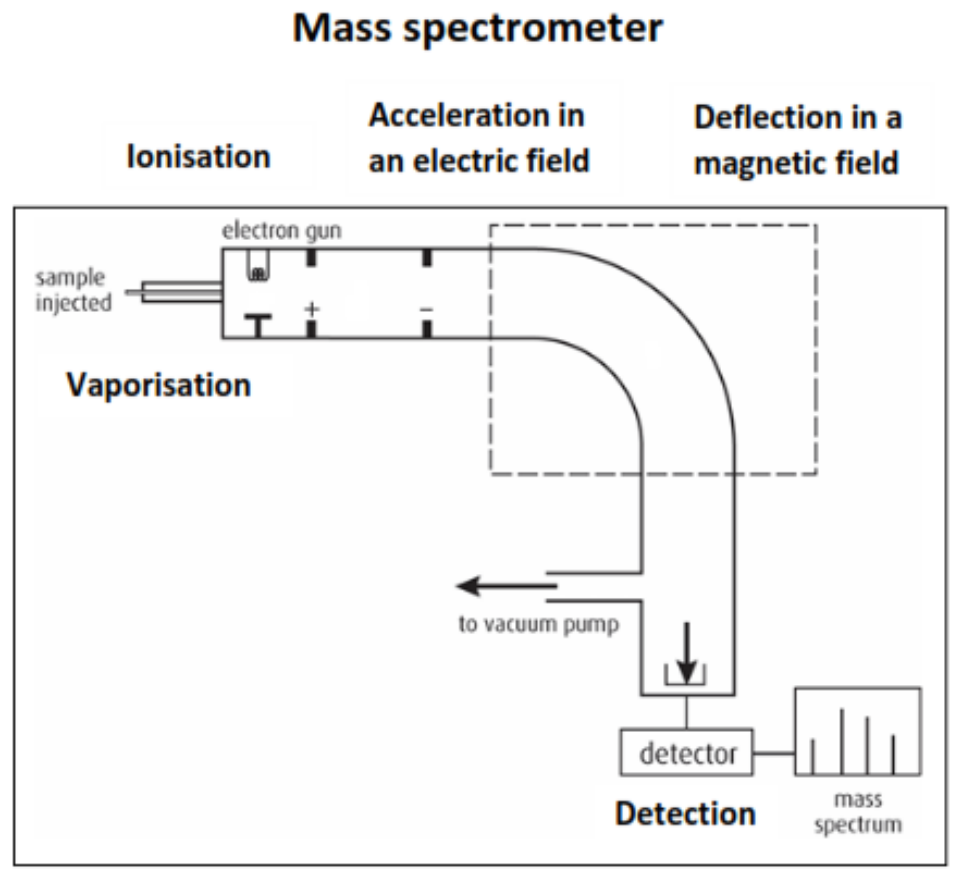
82
Pb
207.20

$$A_r = \frac{(2\times204)+(24\times206)+(22\times207)+(52\times208)}{100} = 207.2$$

MSJChem
Tutorials for IB Chemistry

Mass spectrometry

Mass spectrometry can also be used to determine the structure of a compound.



When the vaporised organic sample passes into the ionisation chamber of a mass spectrometer, it is bombarded by a stream of electrons.

$$M_{(g)} + e^- \longrightarrow M^+_{(g)} + 2e^-$$

The $M^+_{(g)}$ ion is known as the molecular ion.

Mass spectrometry

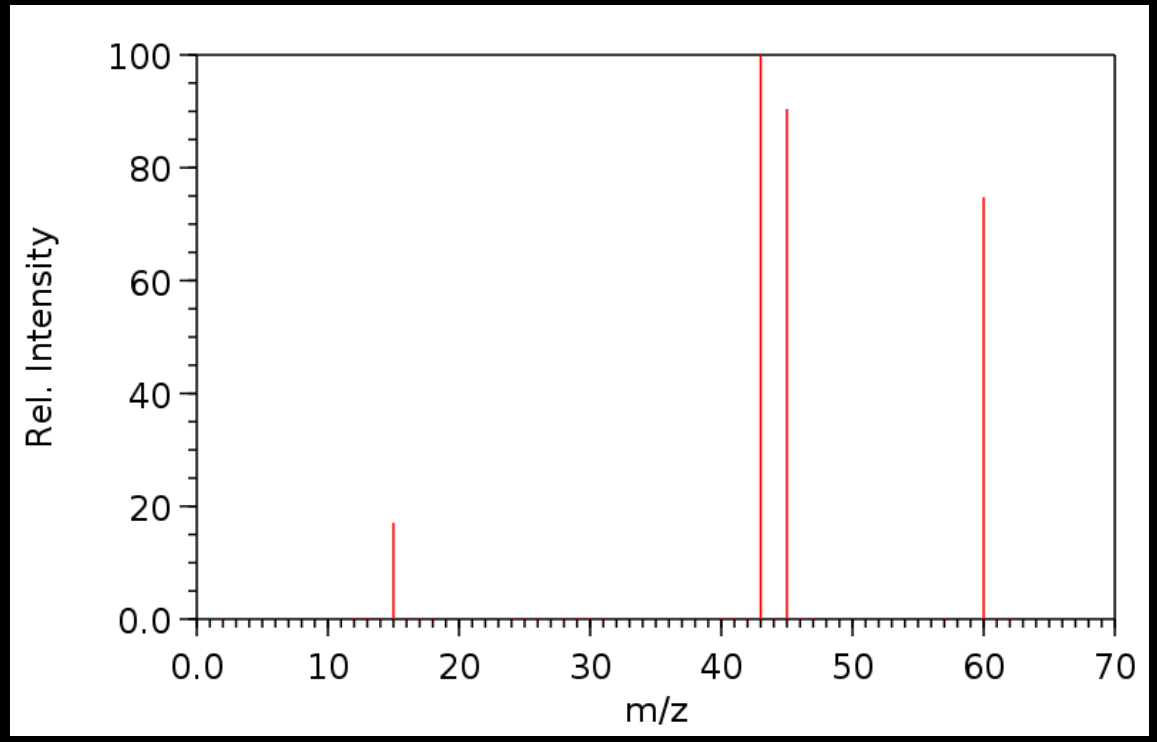
Inside the mass spectrometer, some of the molecular ions break down to produce fragments.

A fragmentation pattern is produced which gives useful information about the structure of the compound.

ethanoic acid

CH_3COOH

$M_r = 60.05$



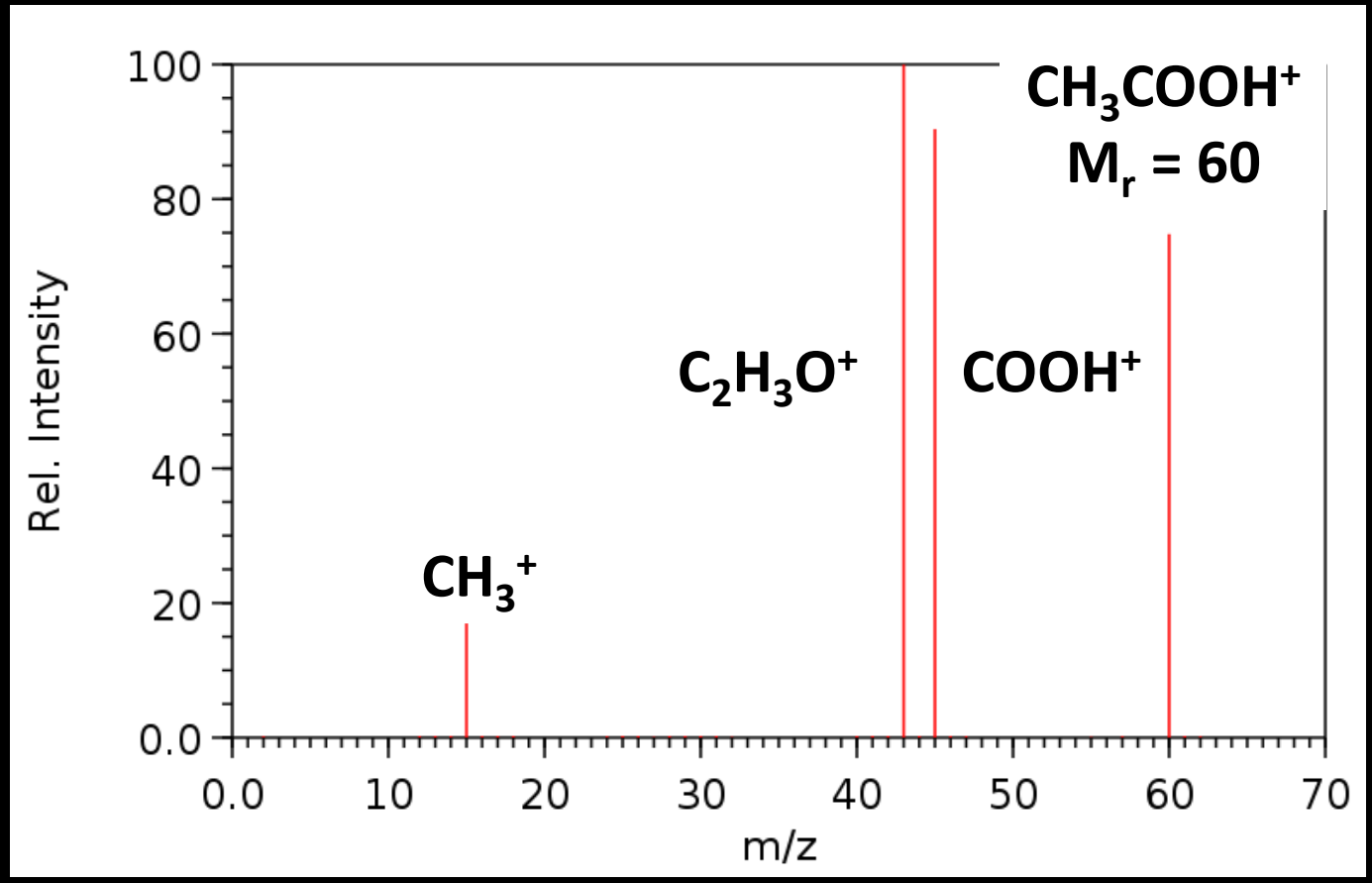
Mass spectrometry

28. Mass spectral fragments lost

Mass lost	Fragment lost
15	CH_3
17	OH
18	H_2O
28	$CH_2{=}CH_2$, C=O
29	CH_3CH_2, CHO
31	CH_3O
45	COOH

MSJChem
Tutorials for IB Chemistry

Mass spectrometry



The peak at m/z = 60 is produced by the molecular ion (M^+)

The peak at m/z = 45 loss of a CH_3 group (60 – 45 = 15)

The peak at m/z = 43 loss of a OH group (60 – 43 = 17)

The peak at m/z = 15 loss of a COOH group (60 – 15 = 45)

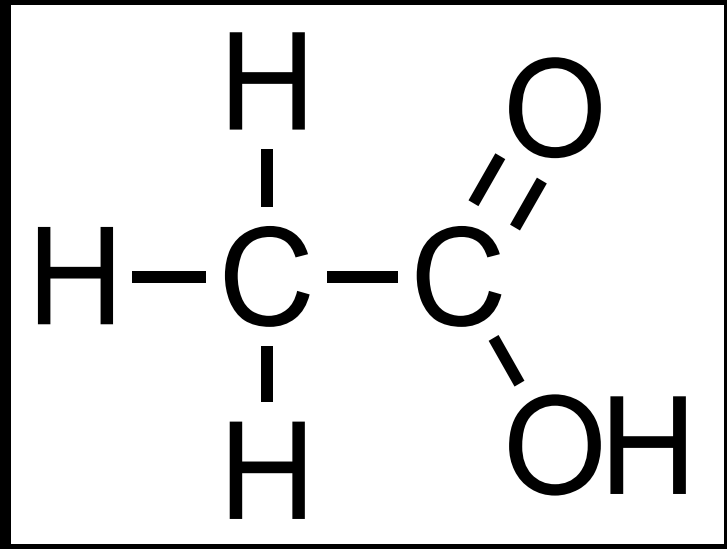
MSJChem
Tutorials for IB Chemistry

Mass spectrometry

Peak	Fragment
45 (60 – 45 = 15)	$COOH^+$ (loss of CH_3)
43 (60 – 43 = 17)	$C_2H_3O^+$ (loss of OH)
15 (60 – 15 = 45)	CH_3^+ (loss of COOH)

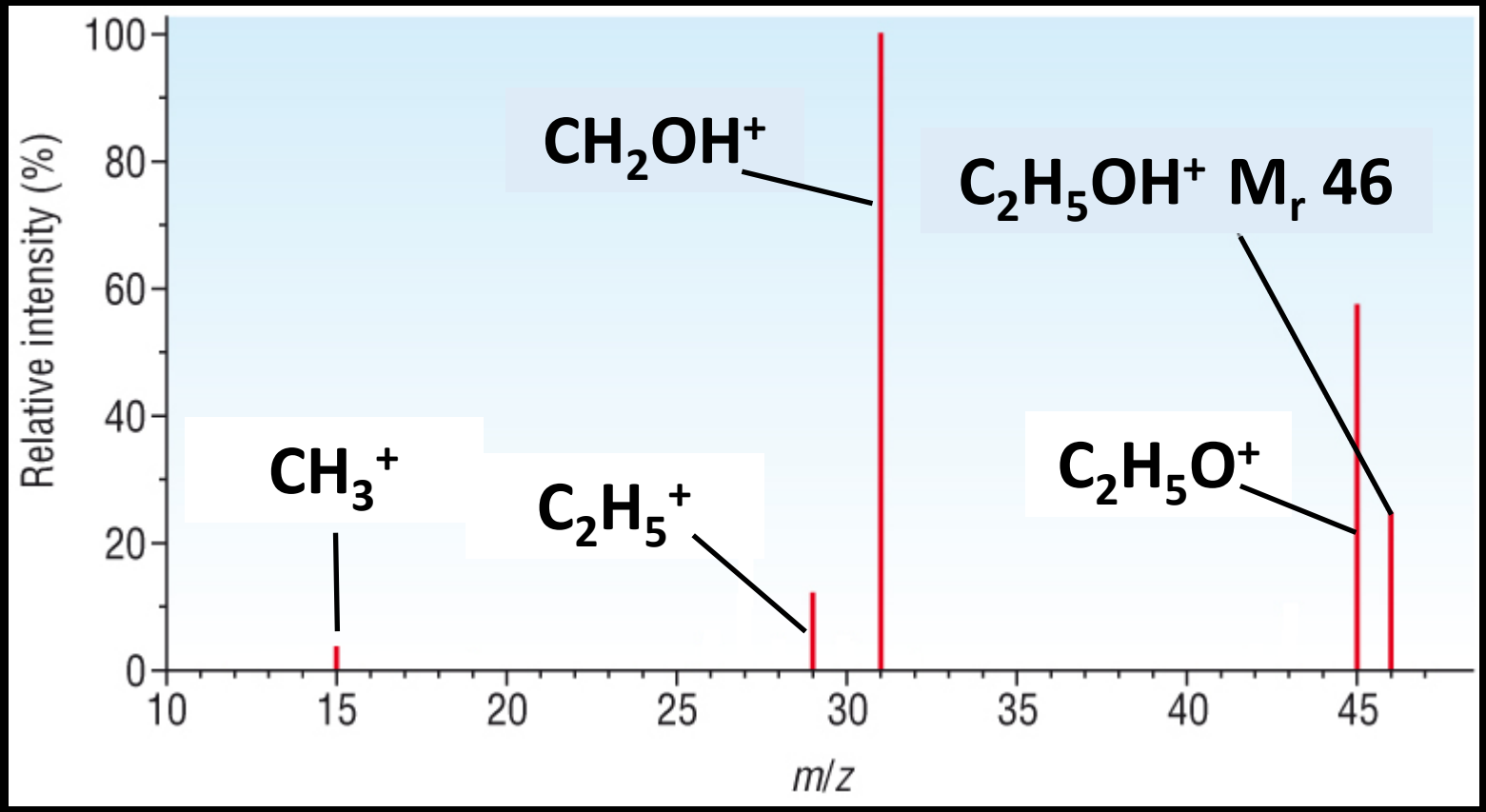
28. Mass spectral fragments lost

Mass lost	Fragment lost
15	CH_3
17	OH
18	H_2O
28	$CH_2=CH_2$, C=O
29	CH_3CH_2, CHO
31	CH_3O
45	COOH



MSJChem
Tutorials for IB Chemistry

Mass spectrometry



The peak at m/z = 46 is produced by the molecular ion (M^+)

The peak at m/z = 45 is produced by the M^+ losing a hydrogen atom (46 – 1 = 45)

The peak at m/z = 31 loss of a CH_3 group (46 – 15 = 31)

The peak at m/z = 29 loss of a OH group (46 – 17 = 29)

The peak at m/z = 15 loss of a CH_3O group (46 – 31 = 15)

MSJChem

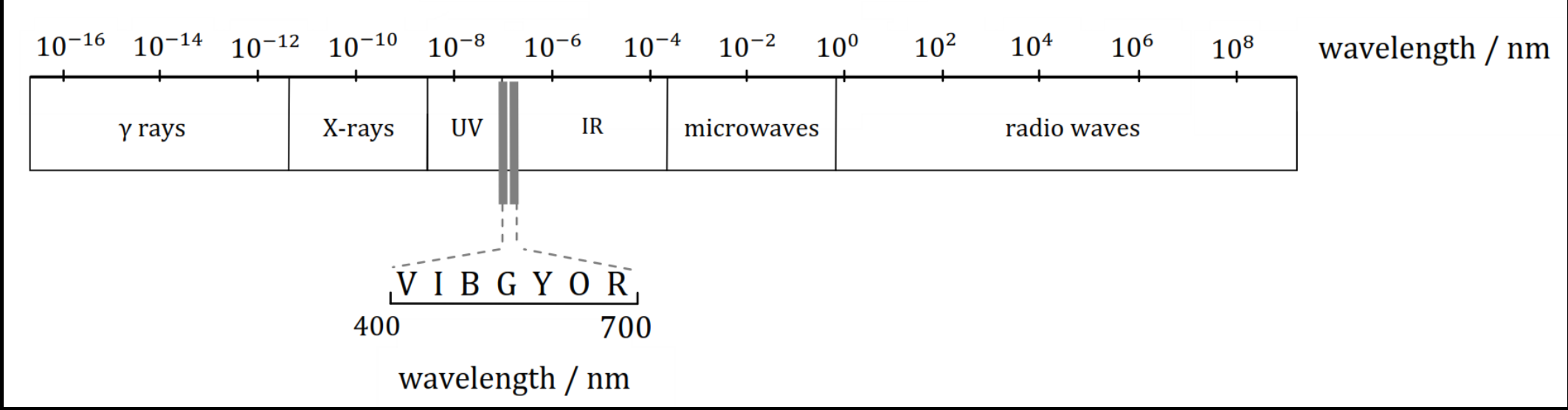
Tutorials for IB Chemistry

Proton nuclear magnetic resonance (^{1}H NMR) spectroscopy

MSJChem
Tutorials for IB Chemistry

^{1}H NMR

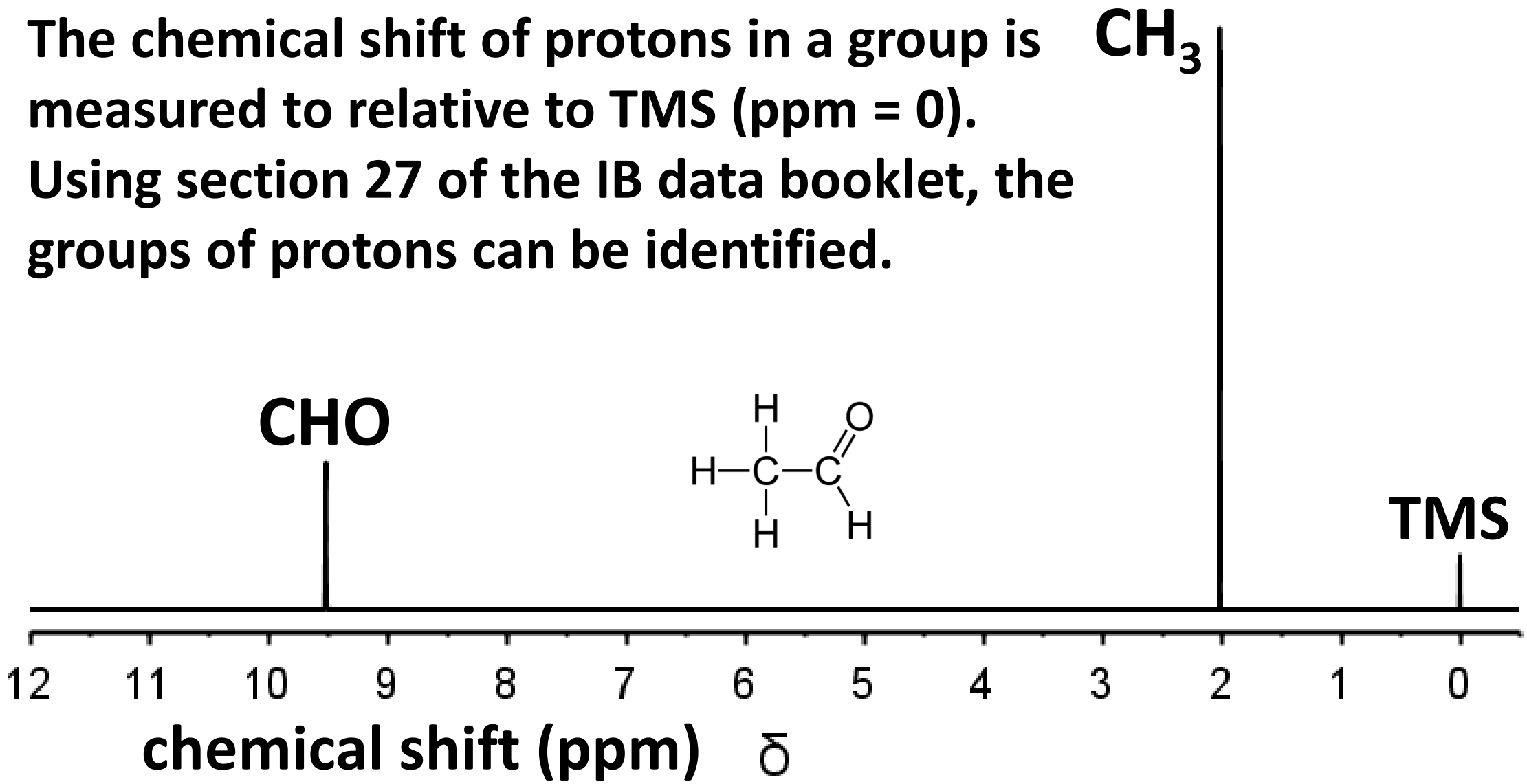
Hydrogen nuclei behave as little magnets and a hydrogen nucleus can be aligned with an external magnetic field or opposed to it (which has higher energy).
The energy needed for the hydrogen nuclei to reverse their spin is very small and can be provided by radio waves.



MSJChem
Tutorials for IB Chemistry

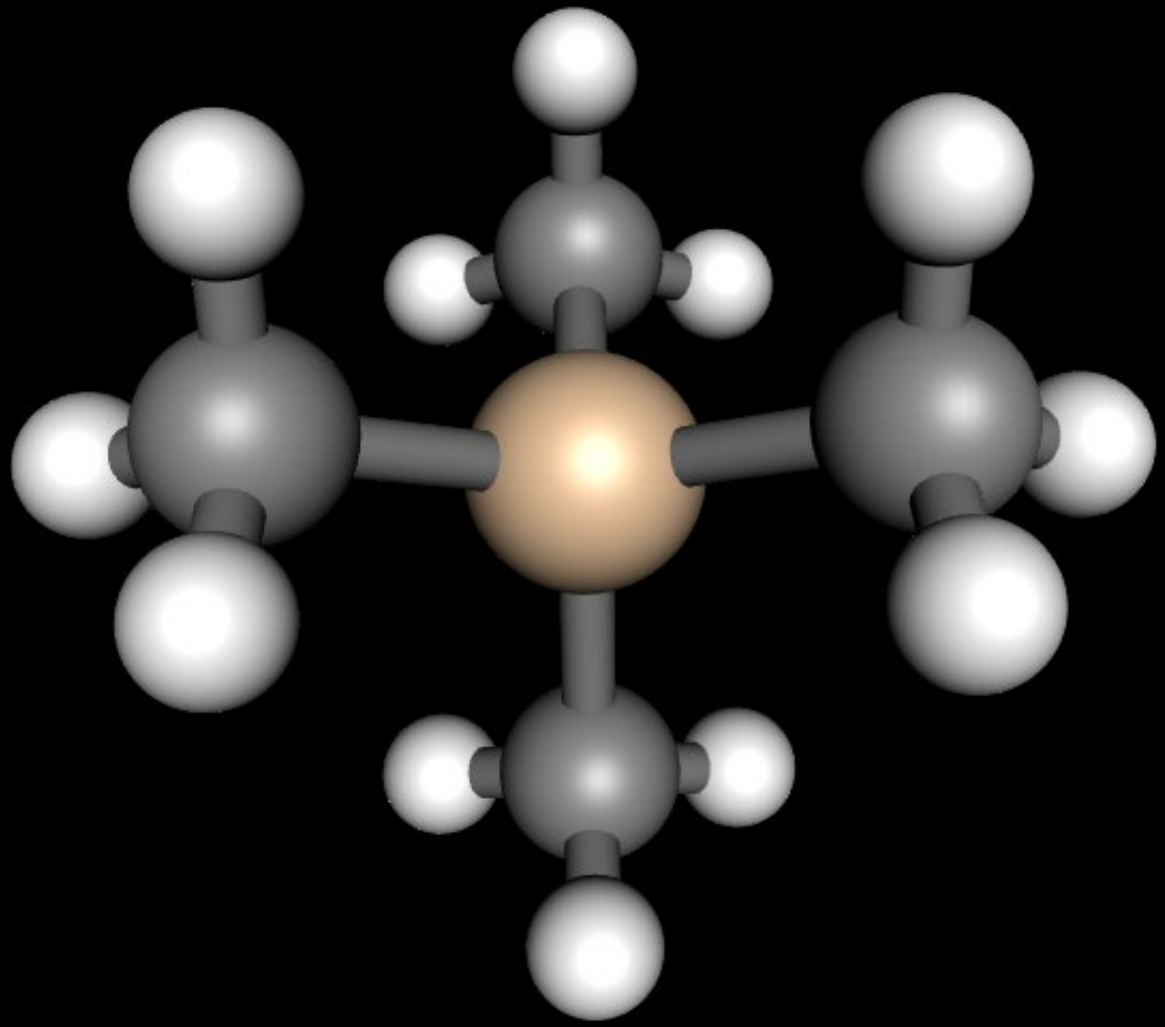
^{1}H NMR

The chemical shift of protons in a group is measured to relative to TMS (ppm = 0). Using section 27 of the IB data booklet, the groups of protons can be identified.



MSJChem
Tutorials for IB Chemistry

^{1}H NMR



The position of the NMR signal is measured relative to the signal produced by TMS tetramethylsilane $Si(CH_3)_4$

MSJChem
Tutorials for IB Chemistry

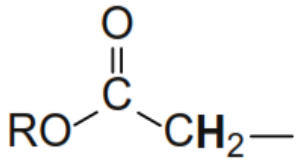
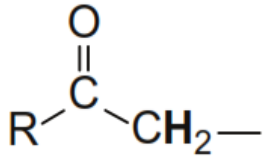
^{1}H NMR

27. ^{1}H NMR data

Typical proton chemical shift values (δ) relative to tetramethylsilane (TMS) = 0.

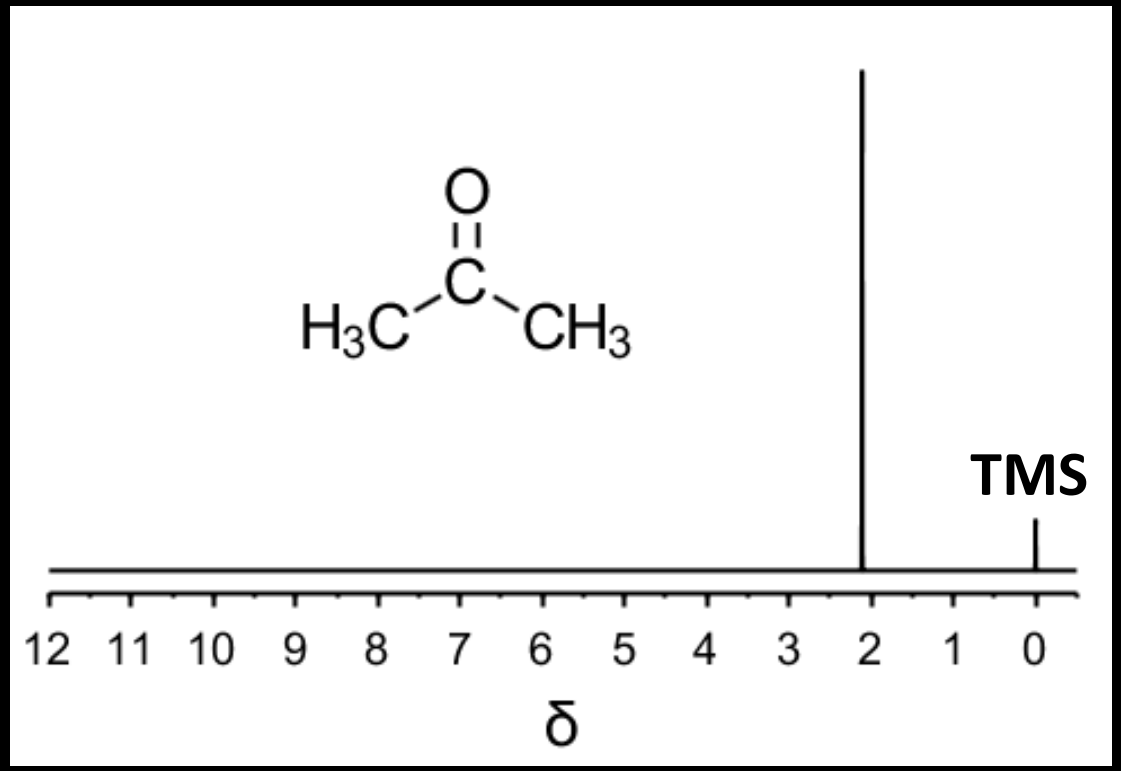
R represents an alkyl group, and Hal represents F, Cl, Br, or I.

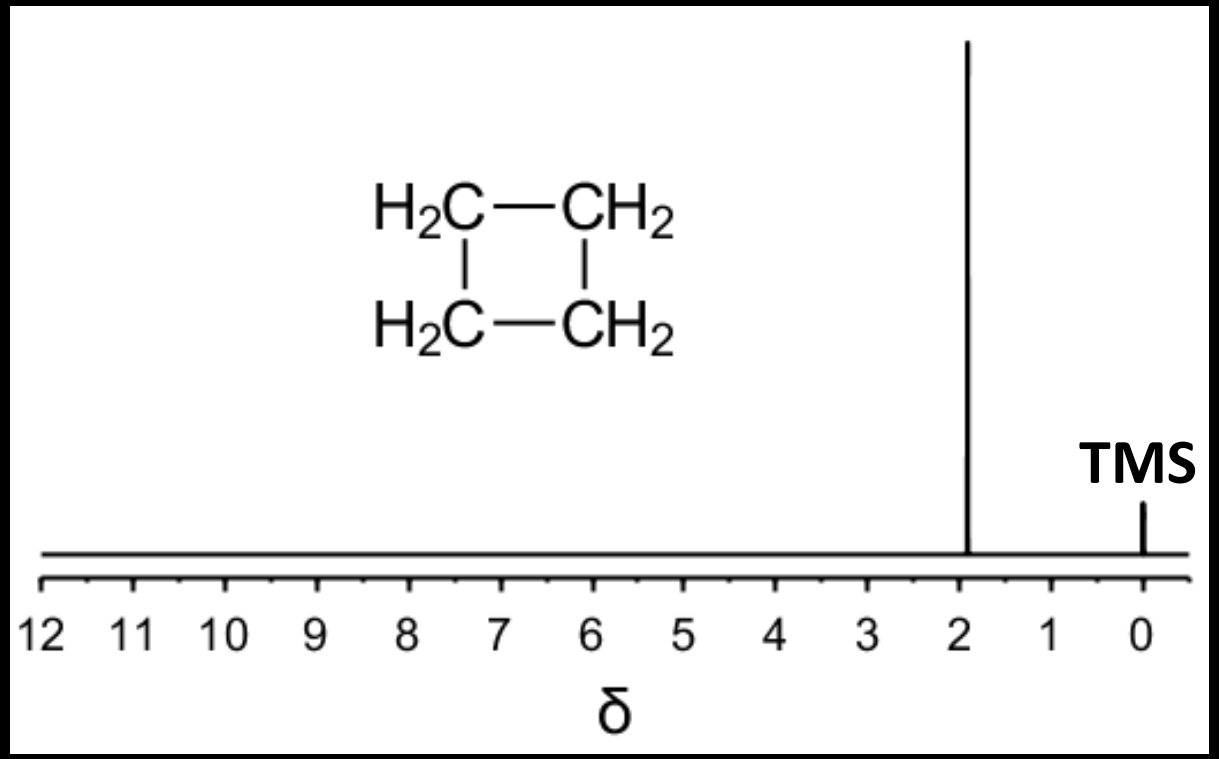
These values may vary in different solvents and conditions.

Type of proton	Chemical shift (ppm)
—C**H**$_3$	0.9–1.0
—C**H**$_2$R	1.3–1.4
—C**H**R$_2$	1.5
	2.0–2.5
	2.2–2.7

MSJChem
Tutorials for IB Chemistry

^{1}H NMR



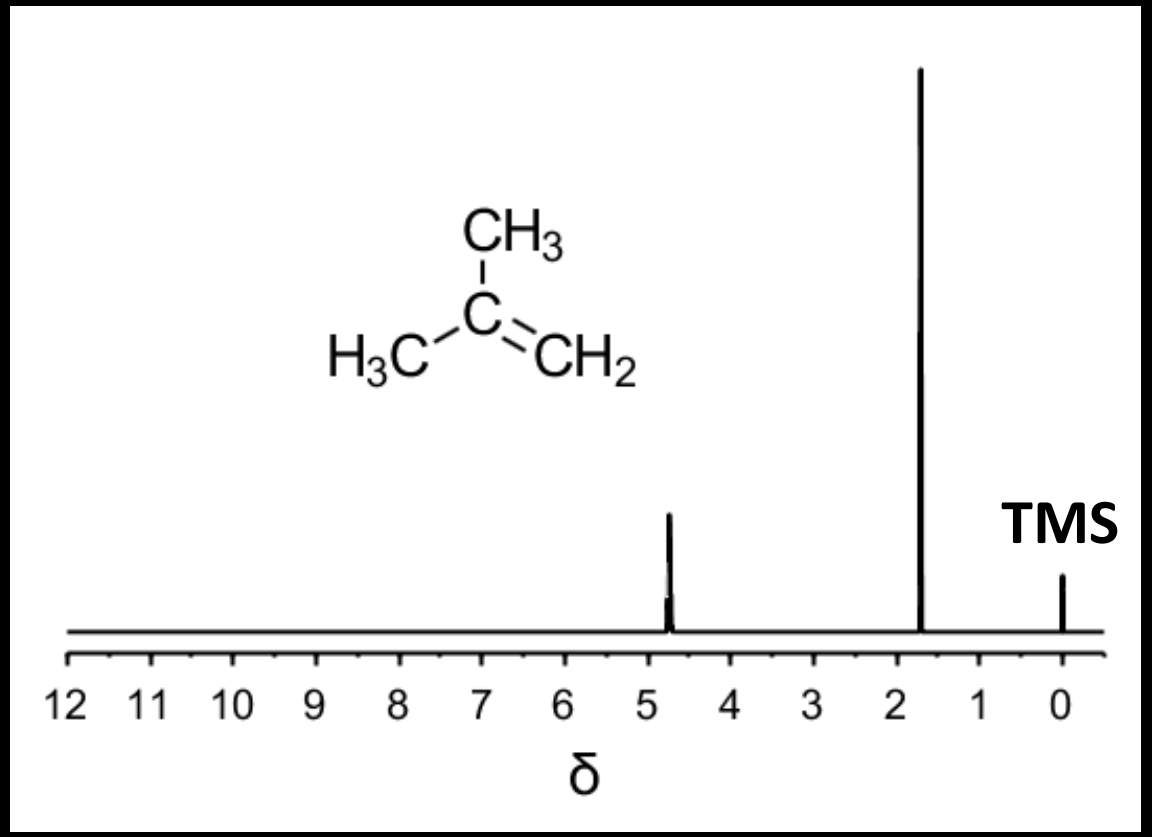


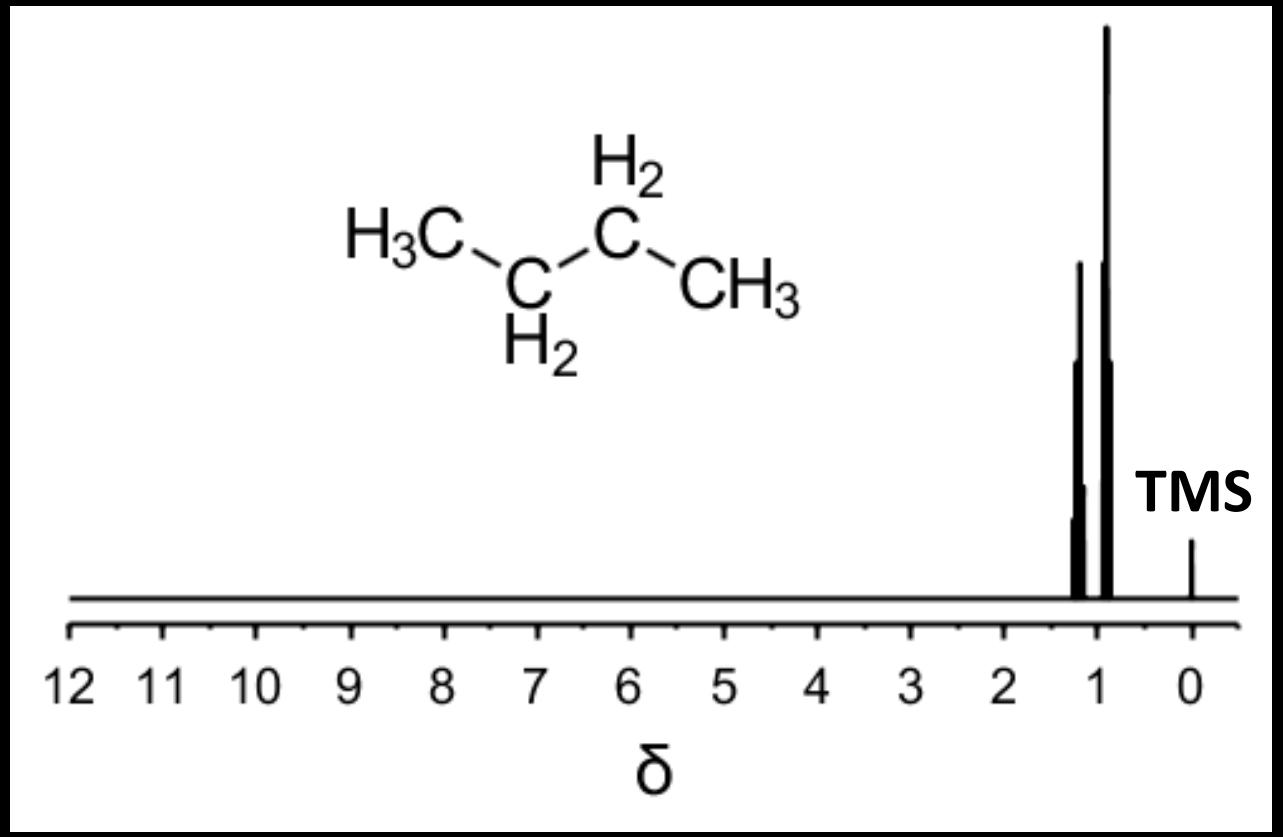
Peak at 2.2 ppm –C**H**$_3$

Peak at 1.9 ppm –C**H**$_2$R

MSJChem
Tutorials for IB Chemistry

^{1}H NMR





Peak at 1.9 ppm –C**H**$_3$

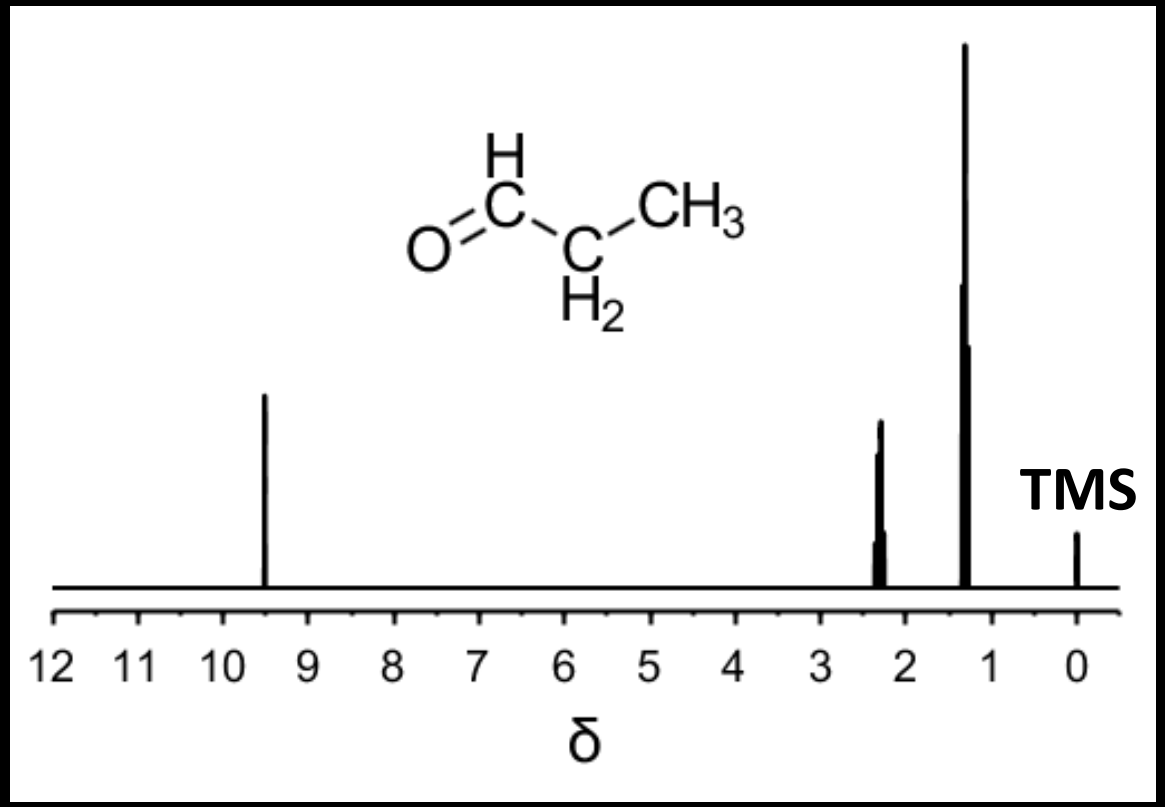
Peak at 4.9 ppm C=C**H**$_2$

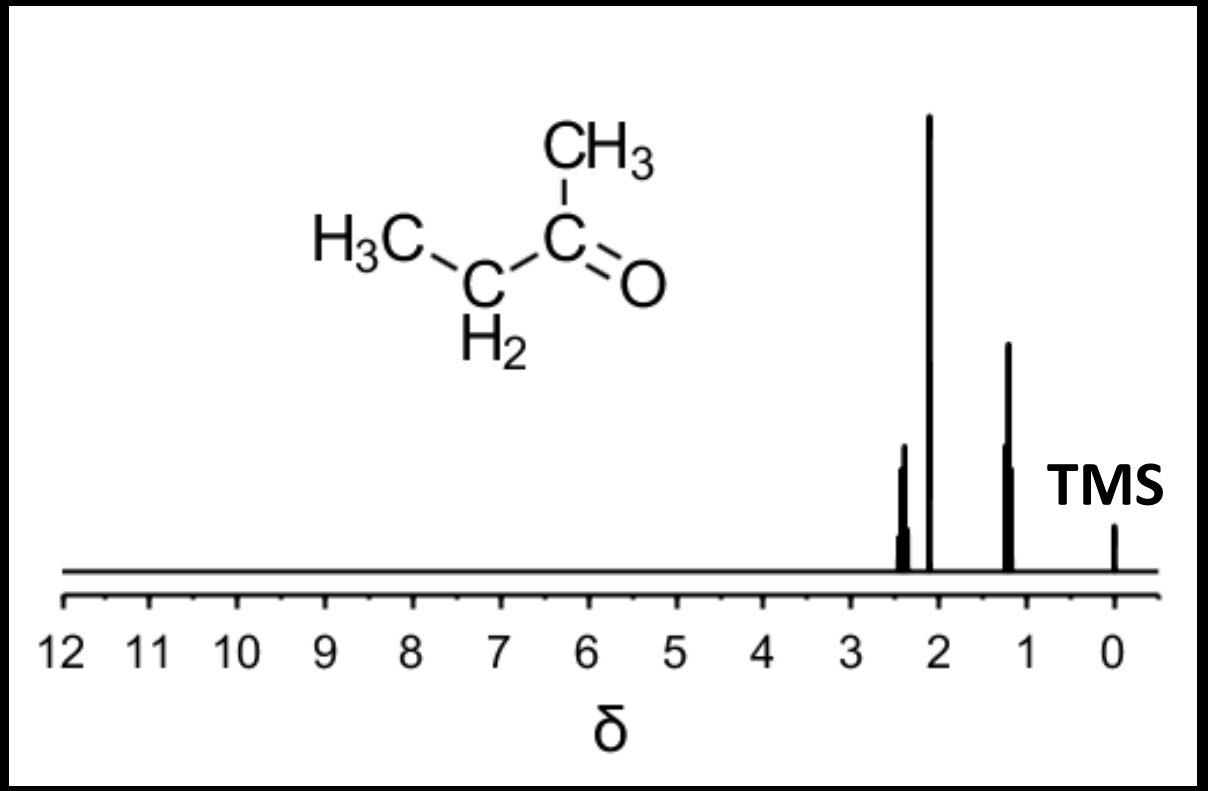
Peak at 0.9 ppm –C**H**$_3$

Peak at 1.3 ppm –C**H**$_2$R

MSJChem
Tutorials for IB Chemistry

^{1}H NMR





Peak at 1.3 ppm –C**H**$_3$
Peak at 2.3 ppm –C**H**$_2$R
Peak at 9.5 ppm R–C**H**O

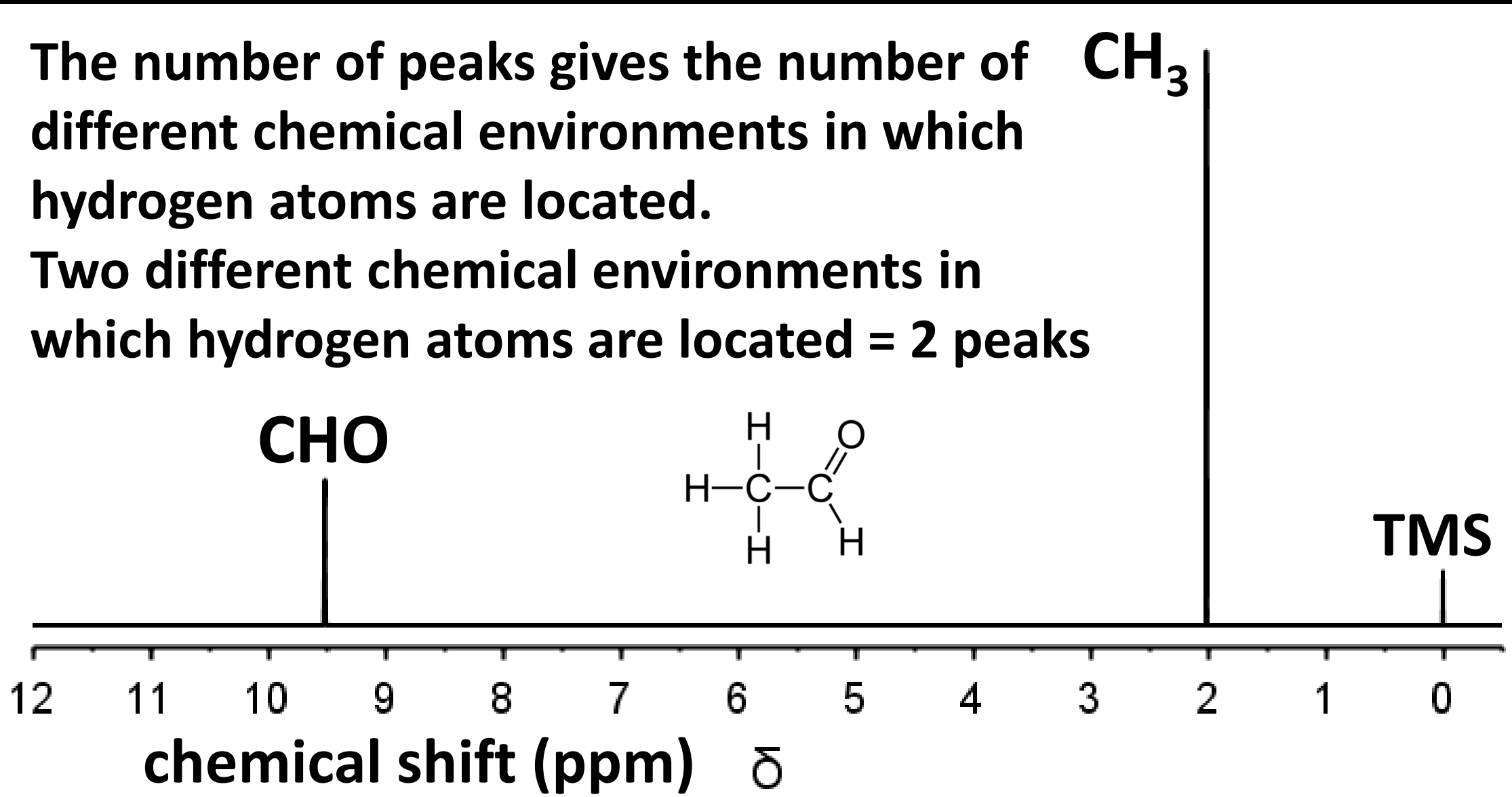
Peak at 1.2 ppm –C**H**$_3$
Peak at 2.1 ppm R–CO–C**H**$_3$
Peak at 2.4 ppm R–CO–C**H**$_2$–

MSJChem
Tutorials for IB Chemistry

^{1}H NMR

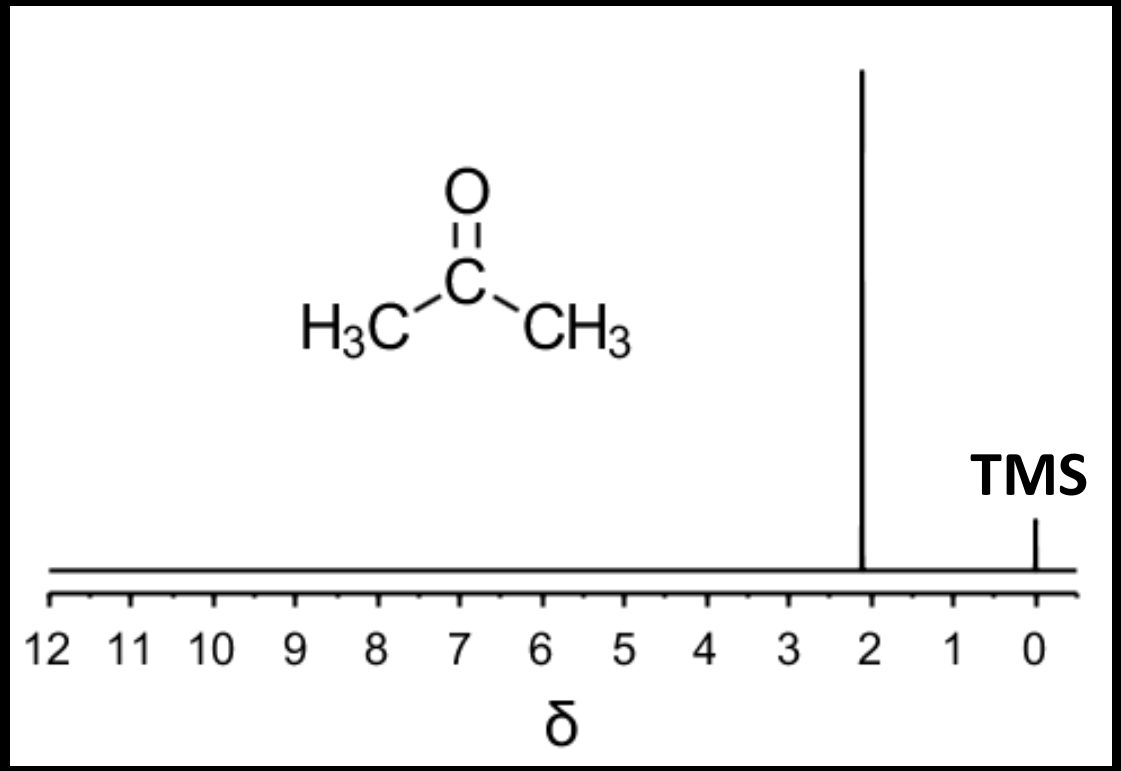
The number of peaks gives the number of different chemical environments in which hydrogen atoms are located.

Two different chemical environments in which hydrogen atoms are located = 2 peaks

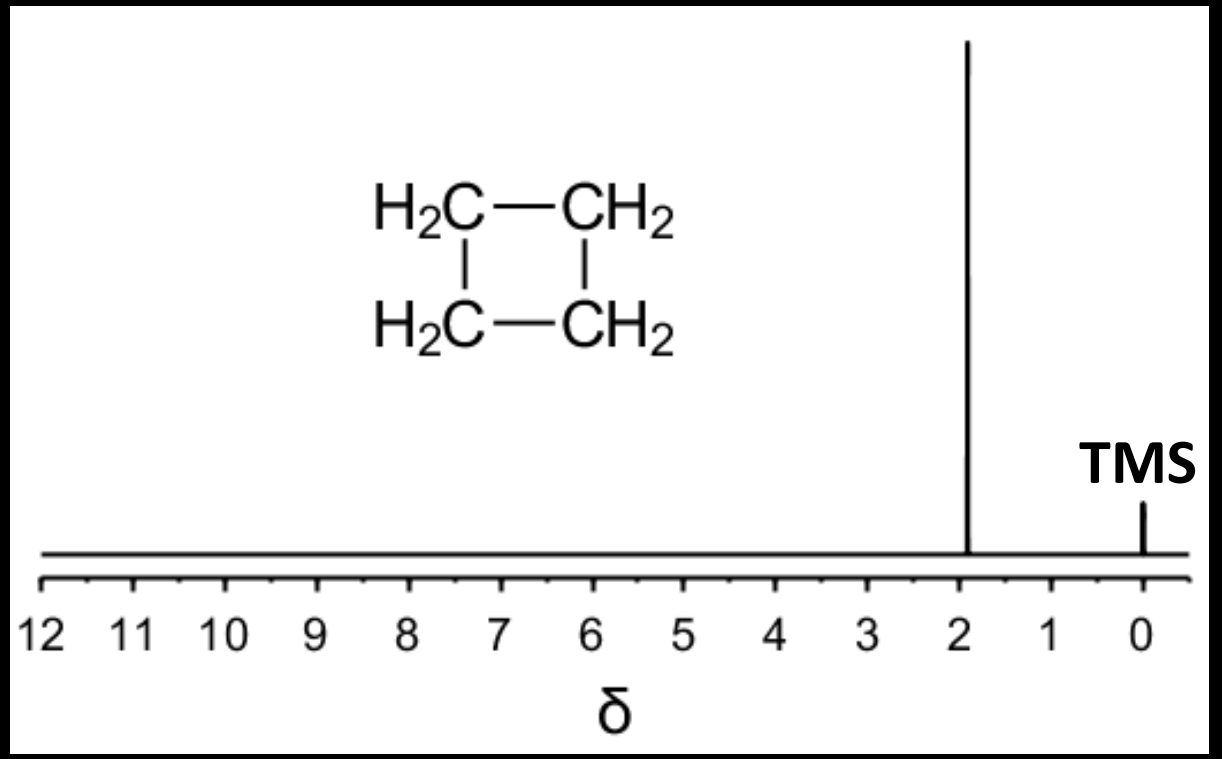


MSJChem
Tutorials for IB Chemistry

^{1}H NMR



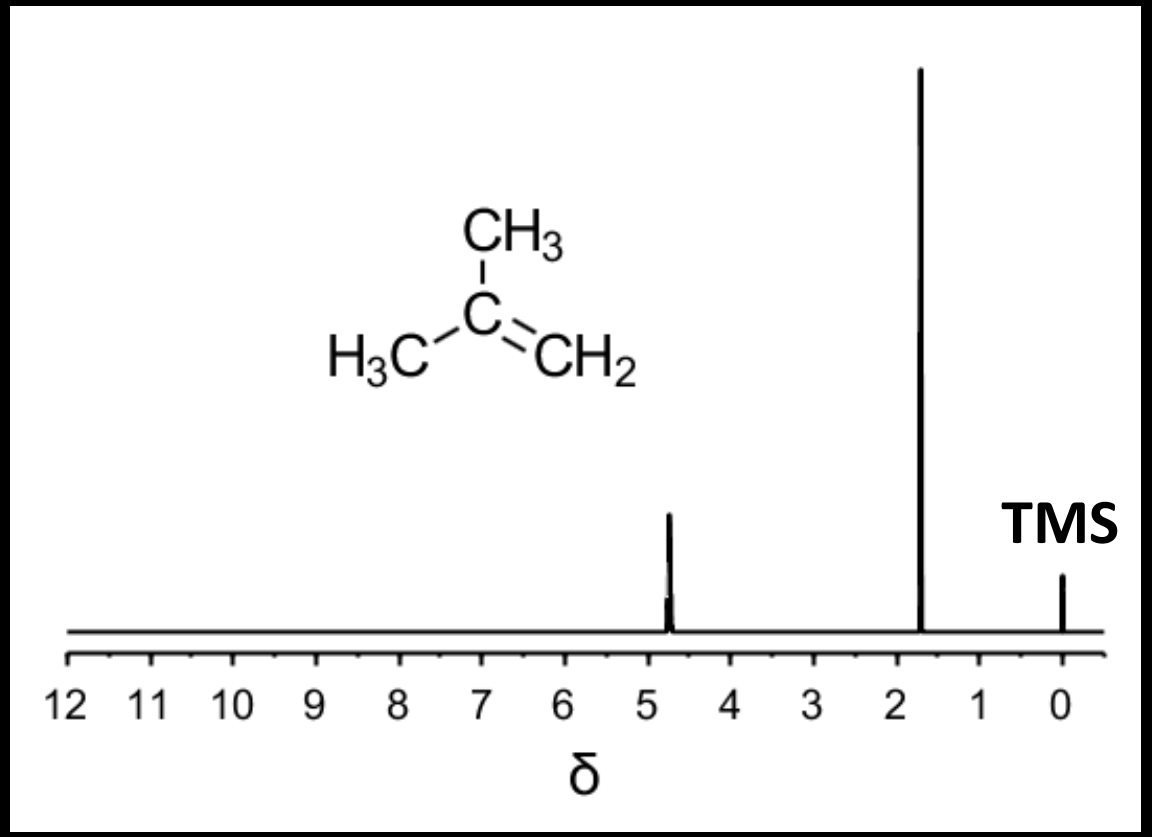
Propanone: Only one type of chemical environment in which hydrogen atoms are located = 1 peak.



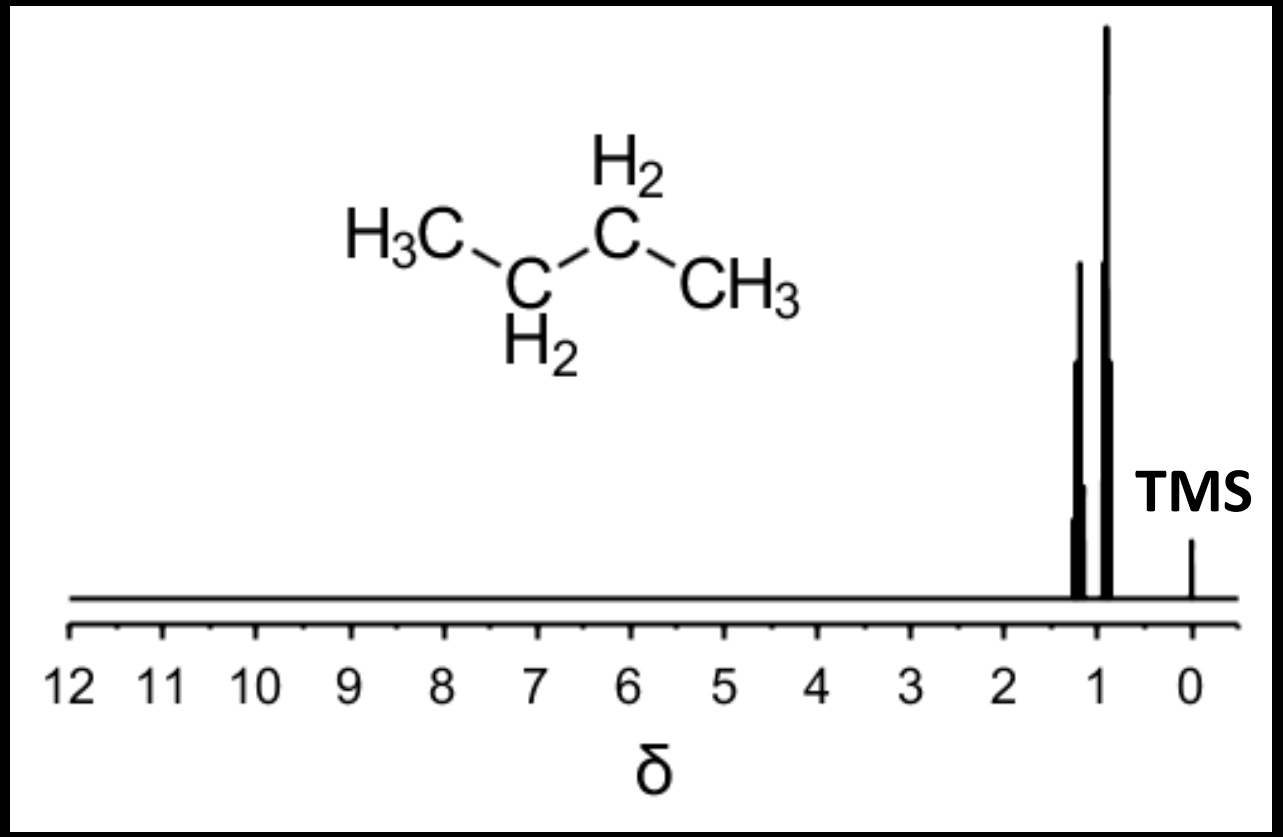
Cyclobutane: Only one type of chemical environment in which hydrogen atoms are located = 1 peak.

MSJChem
Tutorials for IB Chemistry

^{1}H NMR



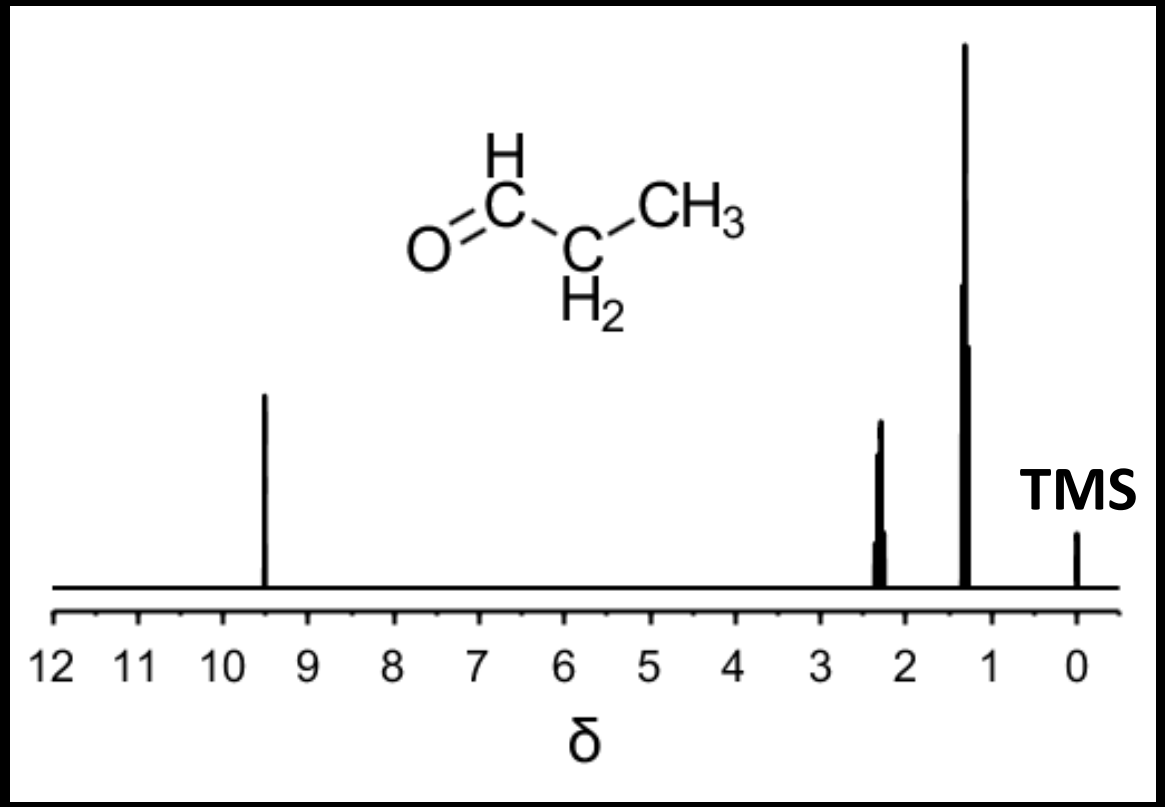
2-methylpropene: two different chemical environments in which hydrogen atoms are located = 2 peaks.



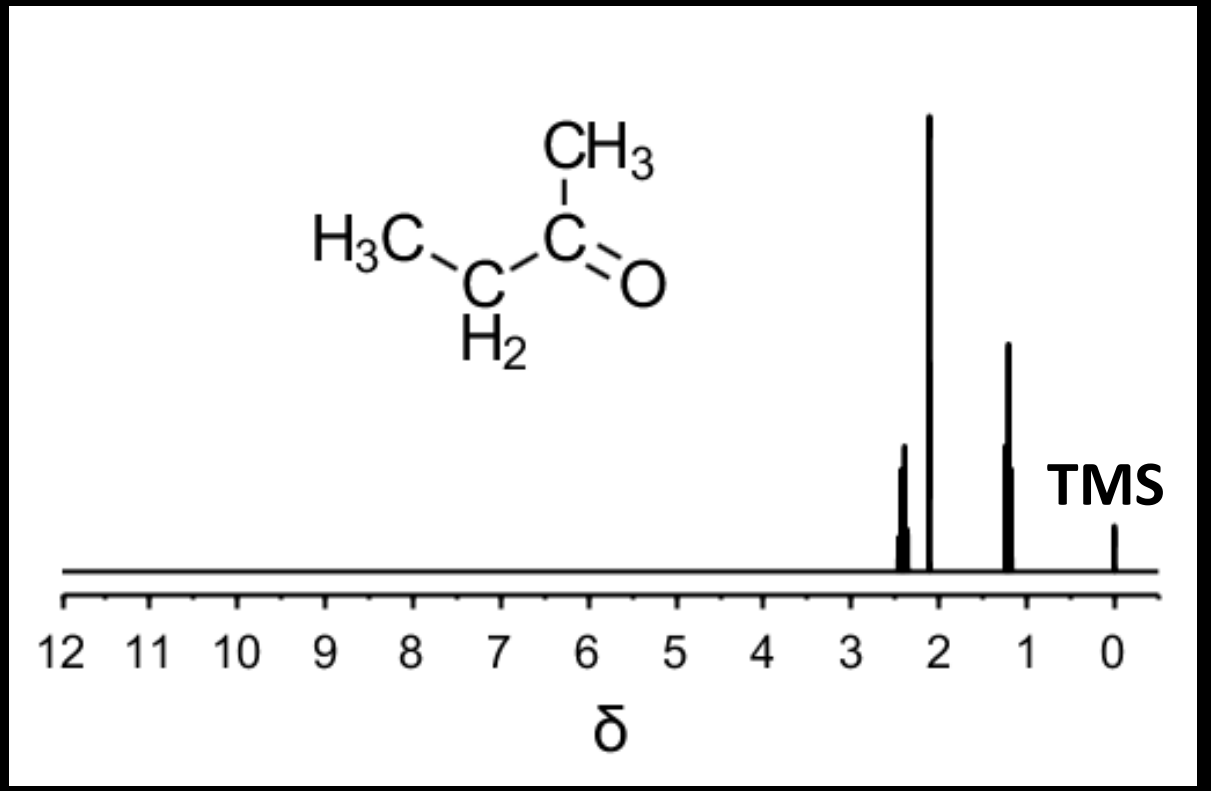
Butane: two different chemical environments in which hydrogen atoms are located = 2 peaks.

MSJChem
Tutorials for IB Chemistry

^{1}H NMR



Propanal: three different chemical environments in which hydrogen atoms are located = 3 peaks.

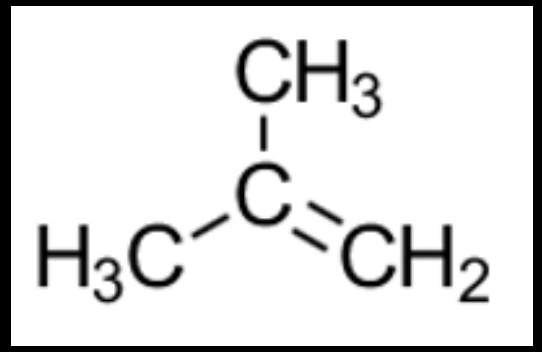


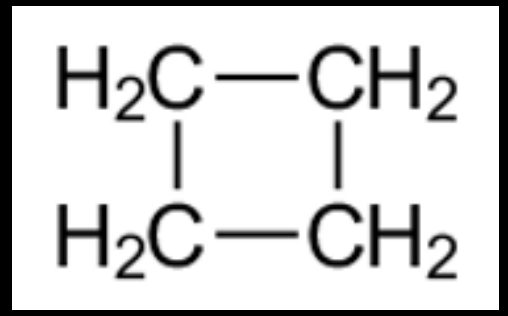
Butanone: three different chemical environments in which hydrogen atoms are located = 3 peaks.

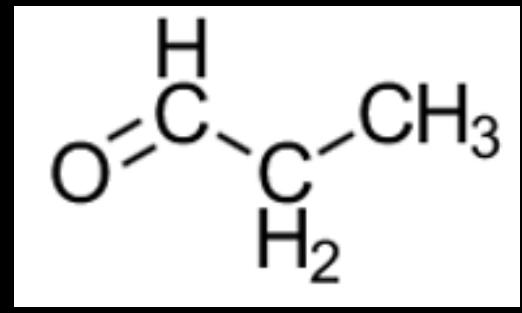
MSJChem
Tutorials for IB Chemistry

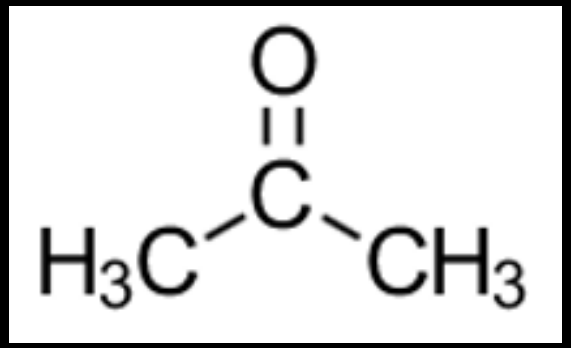
^{1}H NMR

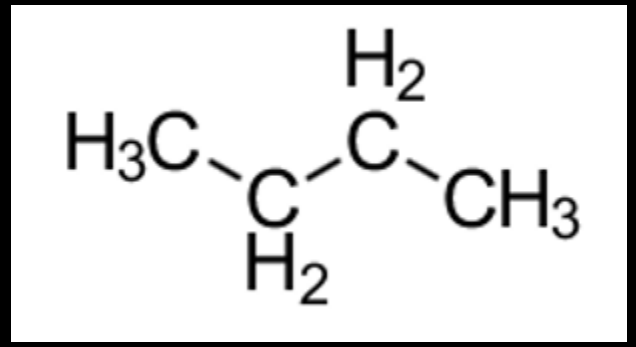
How to determine if hydrogen atoms (protons) are in different chemical environments.

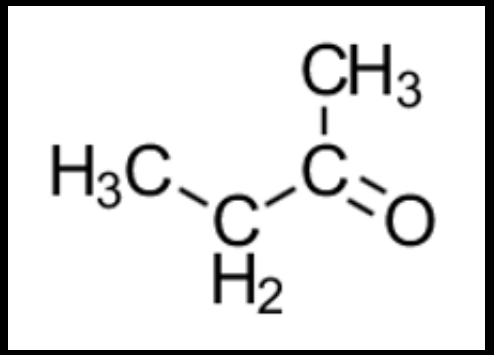






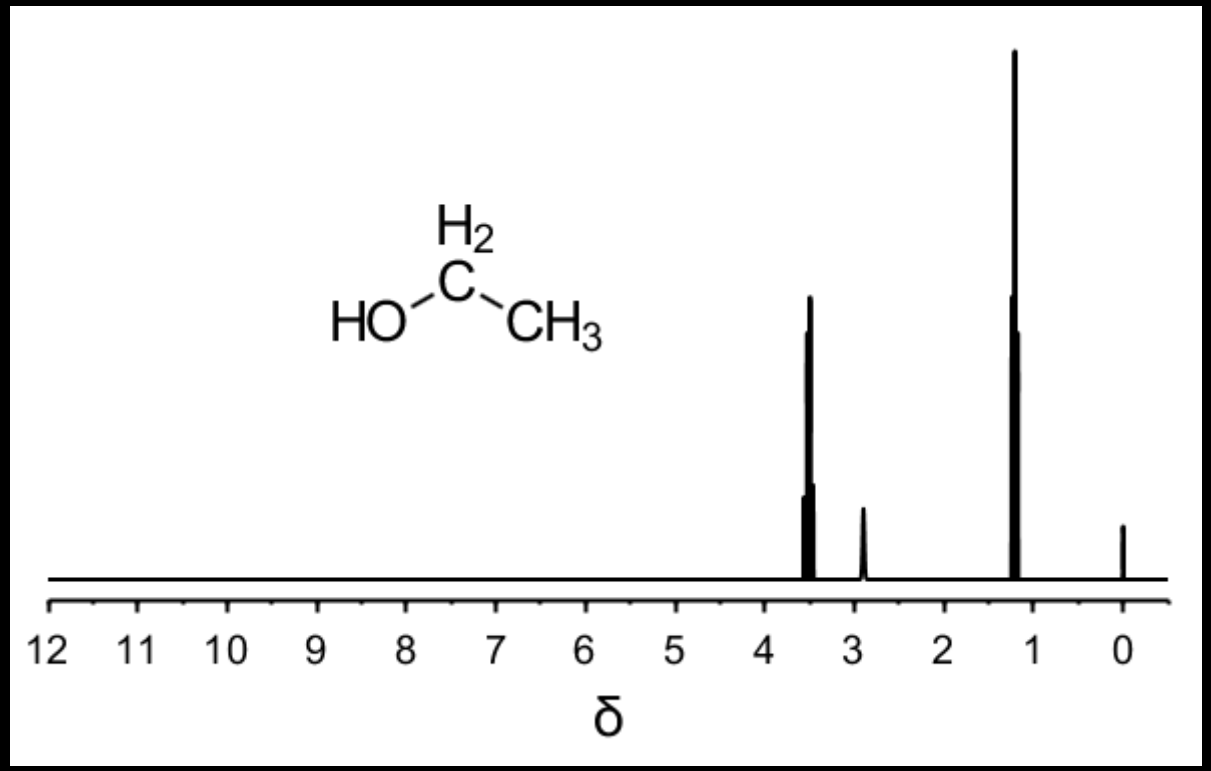


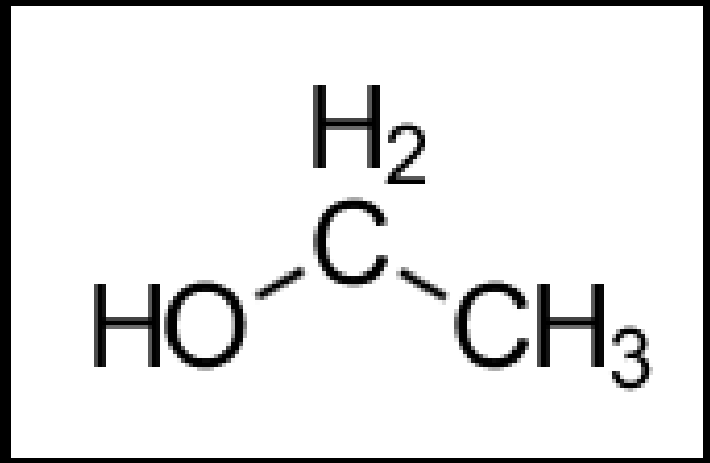




MSJChem
Tutorials for IB Chemistry

^{1}H NMR





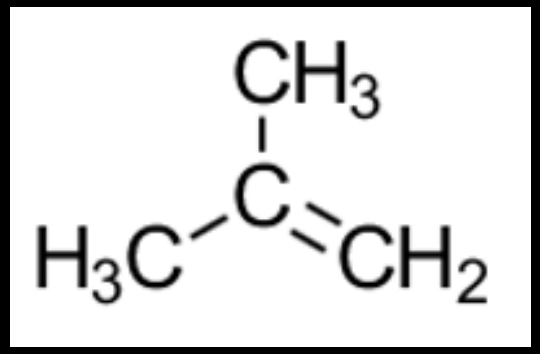
Ethanol: three different chemical environments in which hydrogen atoms are located = 3 peaks.

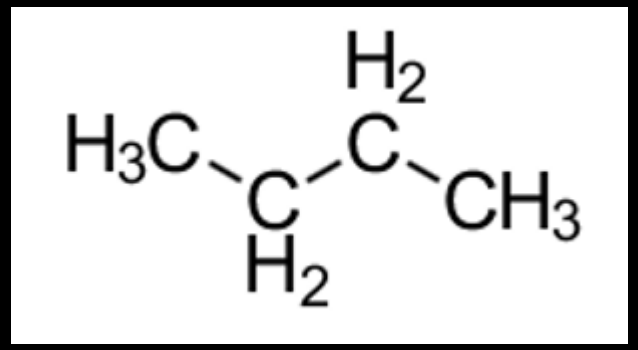
MSJChem
Tutorials for IB Chemistry

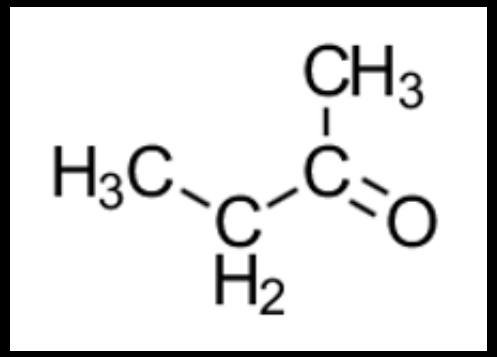
^{1}H NMR

Summary:

- If there are two of the same group (two CH_3 groups), look at the groups of atoms that those groups are bonded to; if they are the same, then the protons are in the same chemical environment, if not, they are in different chemical environments.

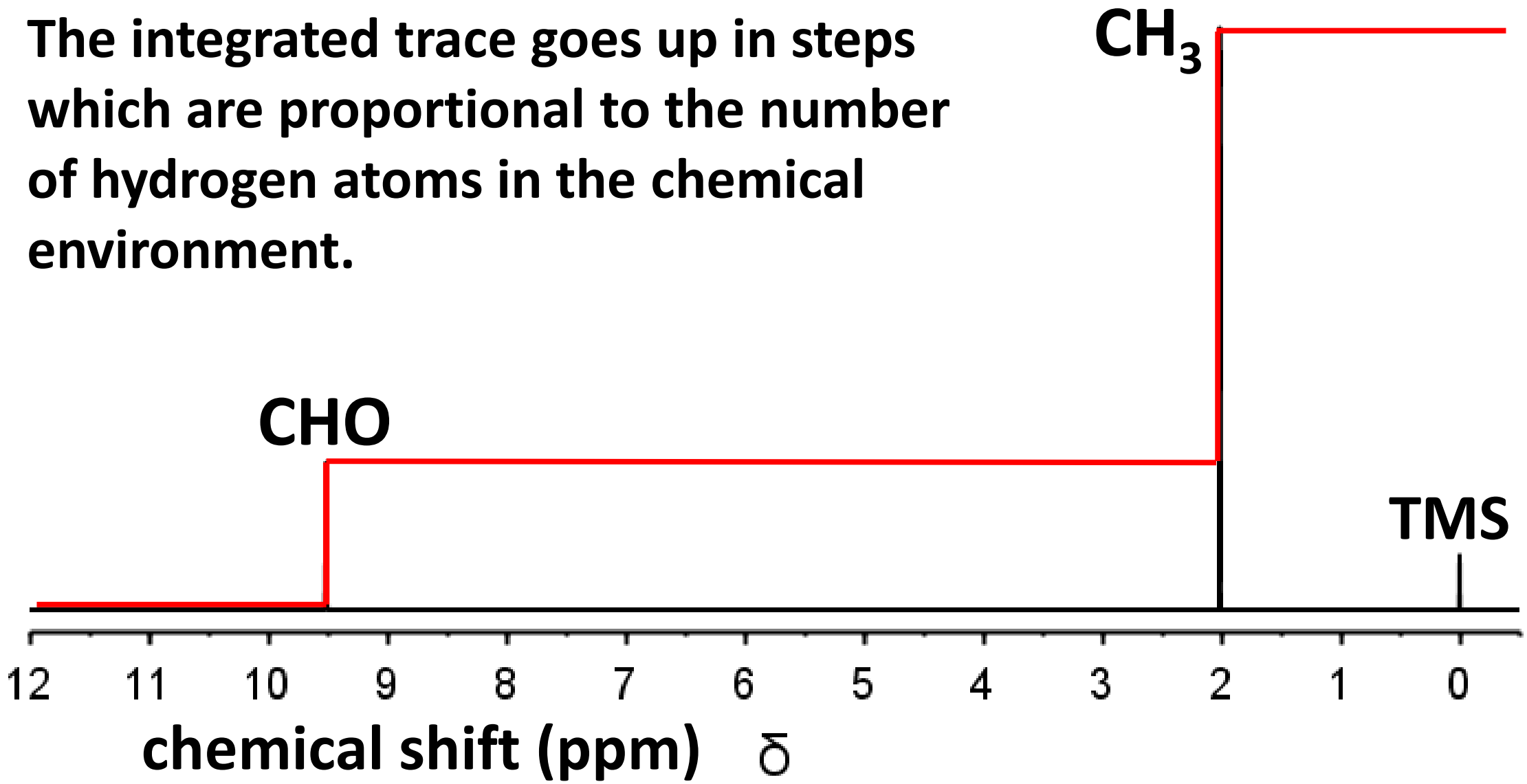






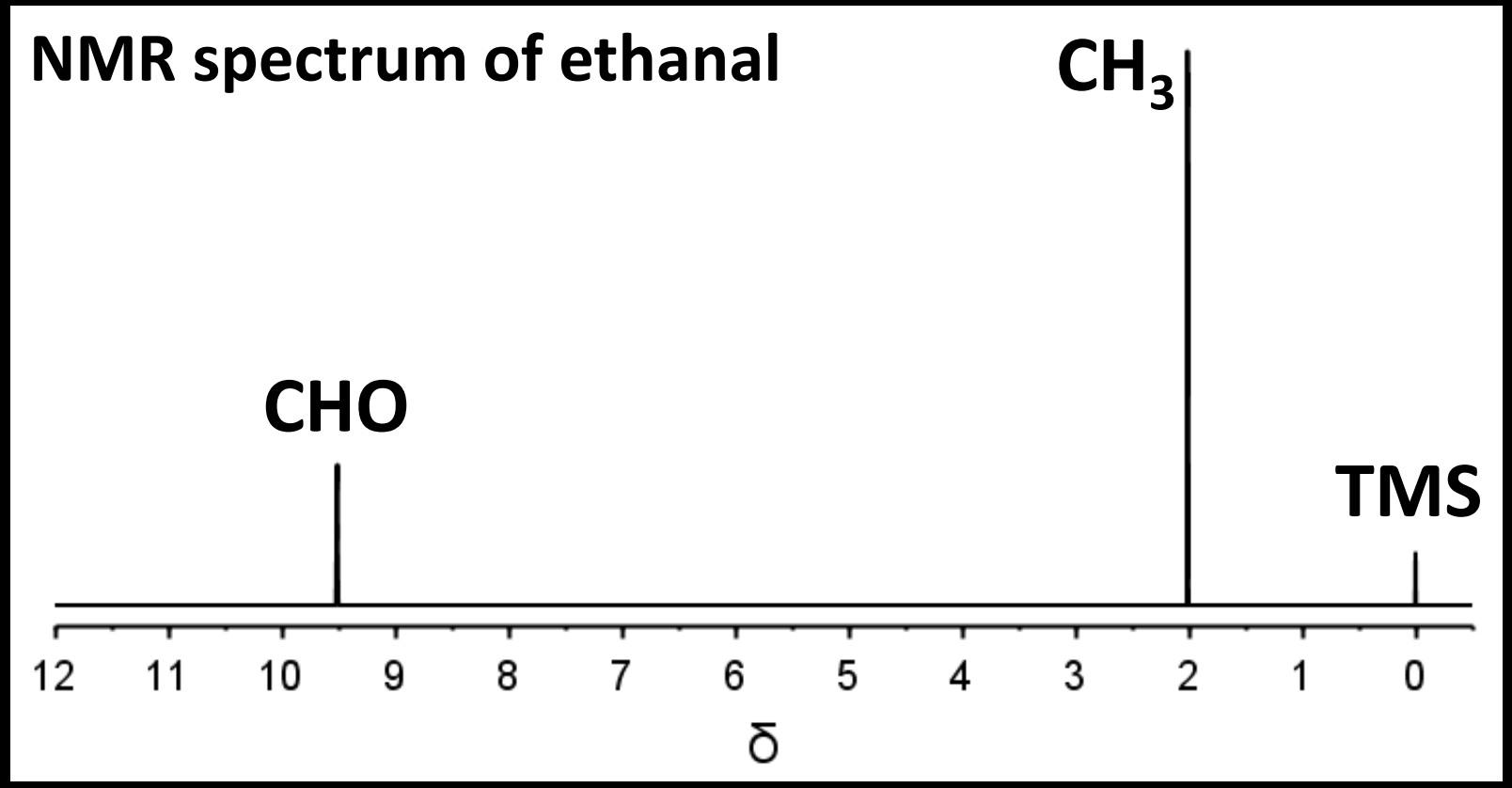
^{1}H NMR

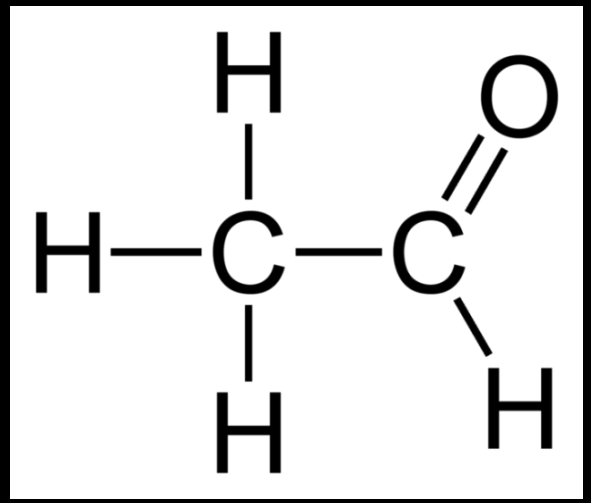
The integrated trace goes up in steps which are proportional to the number of hydrogen atoms in the chemical environment.

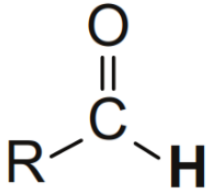


MSJChem
Tutorials for IB Chemistry

^{1}H NMR

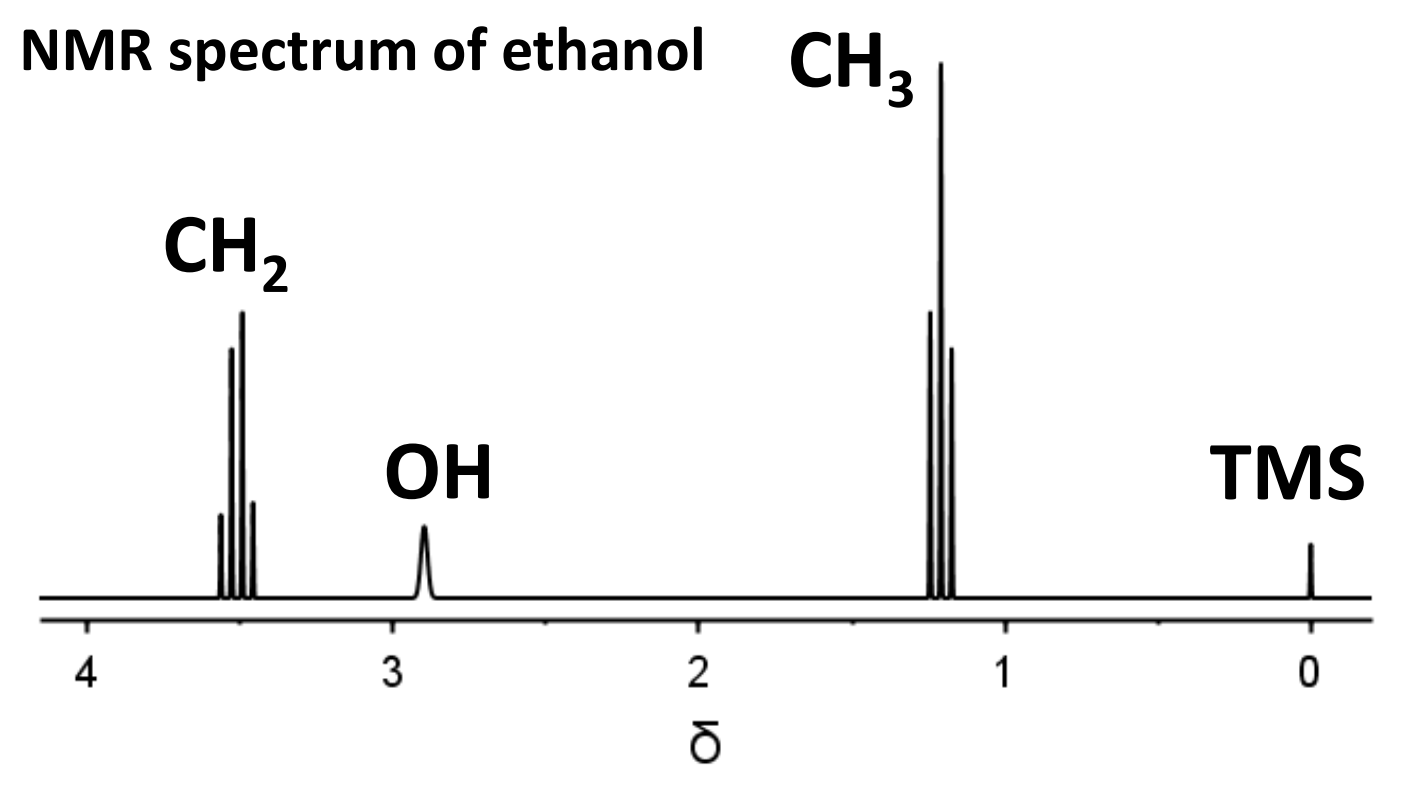


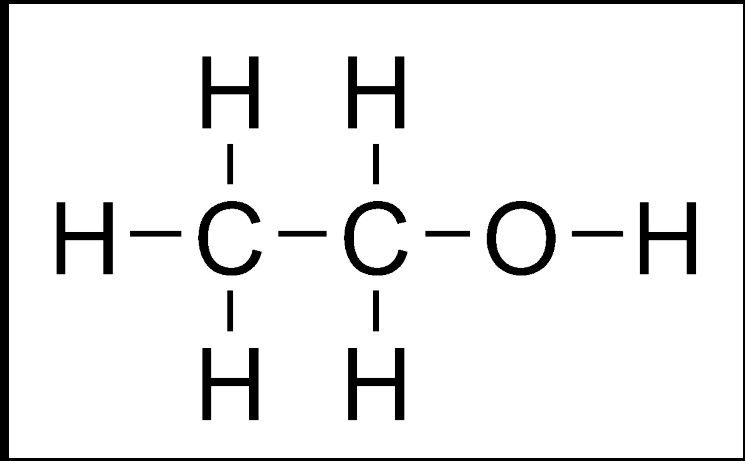


Type of proton	Chemical shift (ppm)
– CH_3	0.9 – 1.0
	9.4 – 10.0

MSJChem
Tutorials for IB Chemistry

^{1}H NMR





Type of proton	Chemical shift (ppm)
– C**H**$_3$	0.9 – 1.0
R–O–C**H**$_2$ –	3.3 – 3.7
R–O–**H**	1.0 – 6.0