An Introduction to Gas Chromatography Mass Spectrometry

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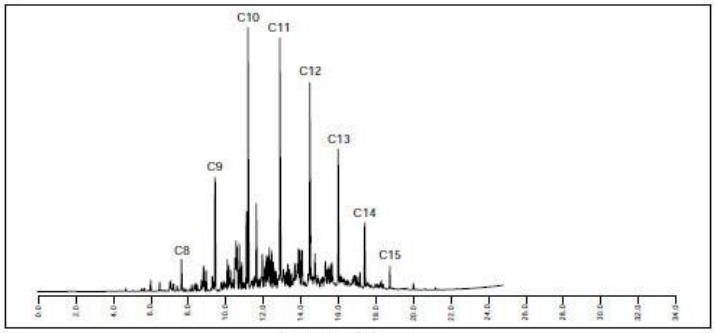
Recommended Textbooks:-

"*Analytical Chemistry*", G. D. Christian, P. K. Dasgupta, K.A. Schug, Wiley, 7th Edition

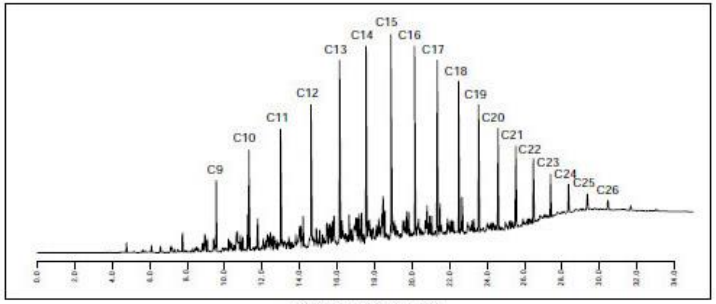
"*Trace Quantitative Analysis by Mass Spectrometry*", R.K. Boyd, C.Basic, R.A. Bethem, Wiley

"*Mass Spectrometry Principles and Applications*", E. de Hoffmann, V. Stroobant, Wiley

GC applications



Analysis of Kerosene



Analysis of Light Oil


GC–MS: The Superior Forensic Tool

Stephen Harrison, Linde Gas, Pullach, Germany.

In the wake of the recent dioxin poisoning scare in Europe that sparked import bans on some German farm products, gas chromatography–mass spectrometry (GC–MS) is emerging as the perfect analytical tool for forensic analysis. In fact, its simplicity, sensitivity and effectiveness in separating and identifying components, has made GC–MS one of the most important tools in analytical chemistry today.

Where other analytical techniques fundamentally determine the quantitative issues arising from analysis of a specific sample — answering the question "how much is present?" — GC–MS is one of a very few techniques able to qualitatively identify the actual nature of chemicals in the sample. It answers the question "What molecules are present?"

Of these two questions, in many analytical scenarios the "what?" is actually more important than the "how much?". Conducting quantitative work on a sample with unknown content is fruitless. The qualitative method is especially relevant to research applications and lays the correct foundation for the analysis. Only when it is known which chemicals are present, can the quantitative analysis be performed.

The GC principle is that molecules in a sample separate in the chromatography column because of differences in their chemical properties. The MS breaks components into ionized species and separates these based on their mass-to-charge ratio. This is the great advantage of the combination of GC as the first separation step and the MS as the qualitative detector.

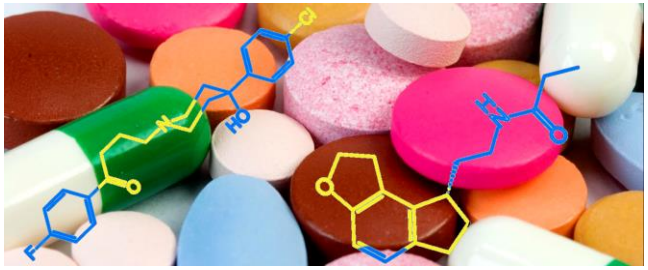
"Amid heightened concerns about food safety in many parts of the world, GC–MS comes to the fore as a very important analytical technique," says the Linde Group's Stephen Harrison, Head of Speciality Gases and Speciality Equipment. "It is one of few techniques to determine exactly what is in a food sample. Characterized by its quick screening abilities, GC–MS has been widely heralded as the 'gold standard' for forensic substance identification."

On the same standing with GC–MS, liquid chromatography–mass spectrometry (LC–MS) is also a qualitative analytical chemistry technique that combines the physical separation capabilities of high performance liquid chromatography with the qualitative analysis capabilities of mass spectrometry. Both techniques involve using a mass spectrometry detector, but GC–MS is used to screen a sample using a gaseous phase component separation process in the gas chromatography column, while LC–MS is able to detect and identify chemicals using a liquid-phase component separation process in the liquid chromatography column.

The medium in which the sample exists and is most effectively separated in the chromatography column — gaseous or liquid — determines which technique is more appropriate. While many samples can be vaporized for

Forensic
Environmental
Food, flavour
Drug development
Energy and fuel

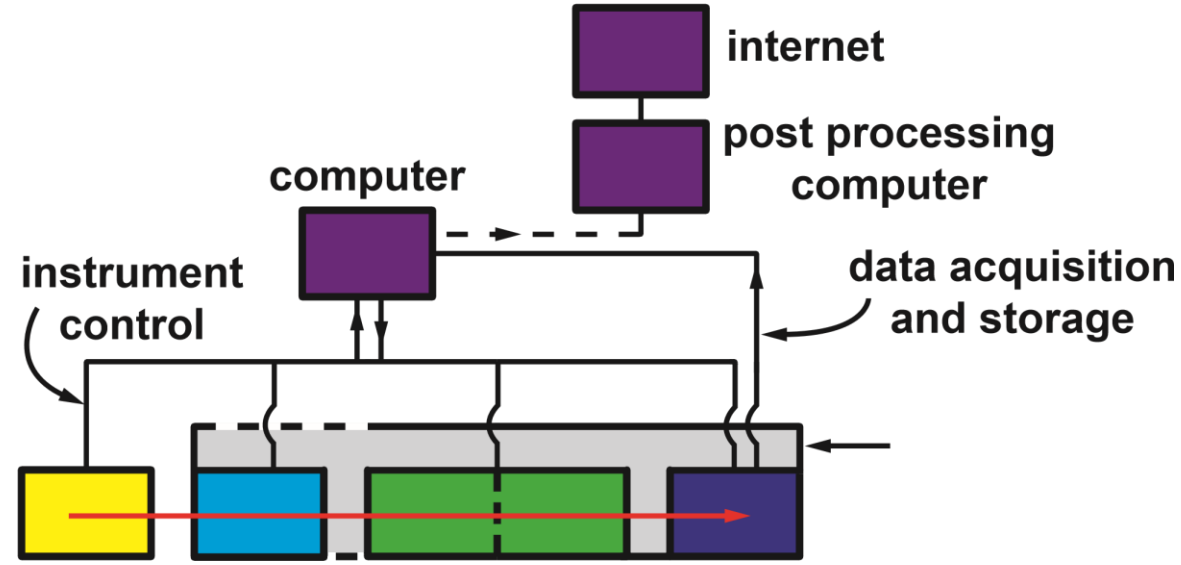
Applications for
Field-Portable GC/MS
in Food Safety



Lecture Overview

- Overview of mass spectrometry instruments
- Mass Spectrometer definition
- Gas Chromatography mass spectrometry instrument overview
- Fundamentals of Chromatographic Separation
  - Principles of chromatographic separations
  - Classification of chromatographic techniques
  - Adsorption chromatography
  - Partition chromatography
  - Gas chromatography (GC)
- Theory of column efficiency in chromatography
  - Rate theory of chromatography - the Van Deemter equation
  - GC mobile phase
  - Retention factor efficiency and resolution
  - Resolution in chromatography
- Gas chromatography columns
- Gas chromatography mass spectrometry (GC-MS)
- Ionisation methods
  - Electron Impact Ionisation (EI) /Chemical Ionisation (CI)
- Quadrupole (Q) mass analyser

Block diagram of a mass spectrometer

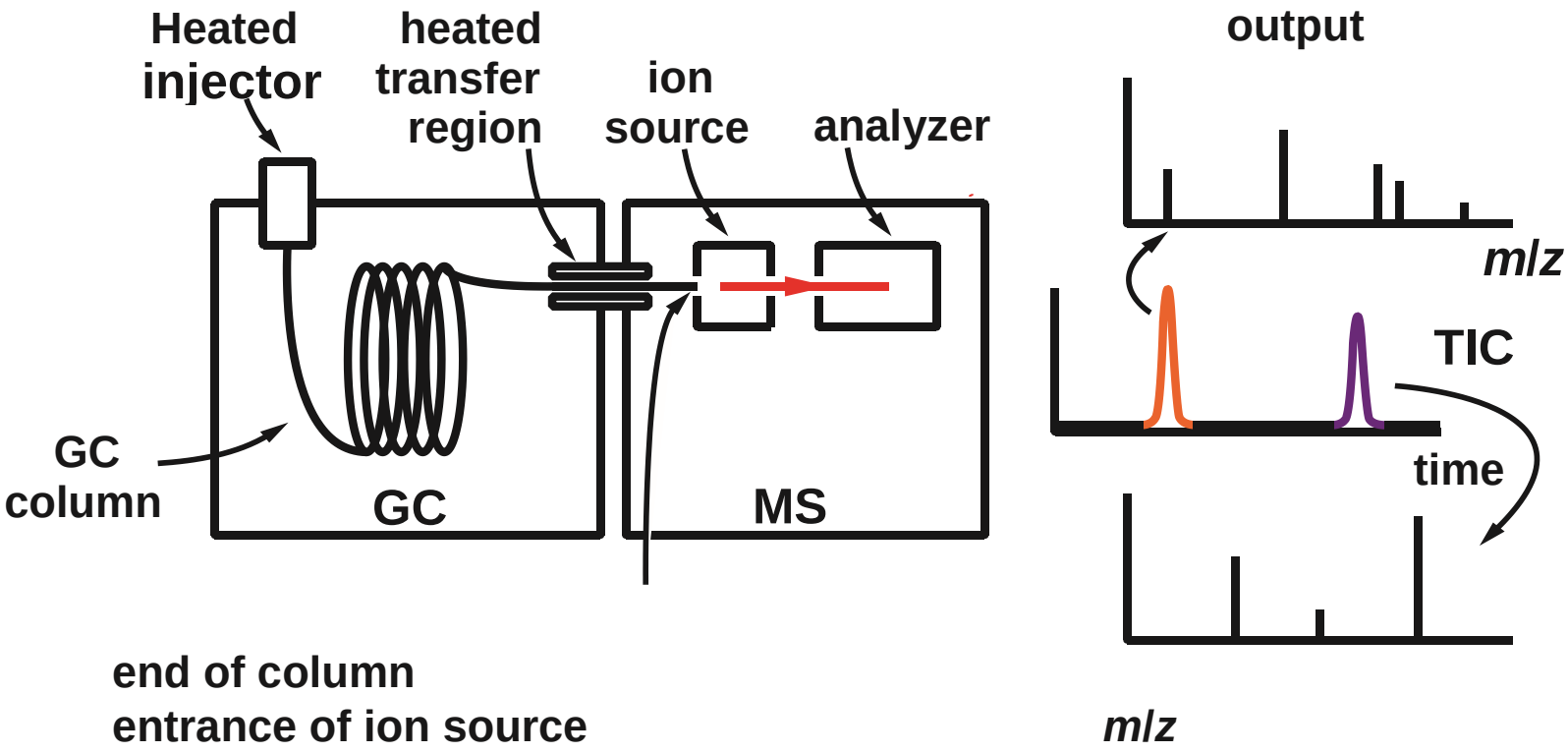


sample inlet	ion source	analyser	detector
GC	EI	Quadrupole	electron multiplier:
LC	CI	ion trap	discrete dynode
CE	APCI	TOF	continuous dynode
gas	APPI	magnetic	MCP
probe	ESI	orbitrap	
	MALDI	ICR	
	DESI		
	DART		

Multiple forms exist for each instrument component, and they can usually be mixed and matched. Analysers can be used in single, e.g., Q or TOF, or in multi-analyser formats, e.g., QTOF and TOF/TOF, with a collision cell incorporated between the two analysers. The computer controls the instrument, acquires data and enables routine data processing, e.g. producing and quantifying spectra.

A mass spectrometer is an analytical instrument that produces a beam of gas ions from samples (analytes), sorts the resulting mixture of ions according to their *mass-to-charge* (*m/z*) ratios using electrical or magnetic fields, and provides analog or digital output signal (peaks) from which the mass-to charge ratio and the intensity (abundance) of each detected ionic species may be determined.

Gas chromatography-mass spectrometer (GC-MS)



Samples are introduced into the GC using a heated injector. Components are separated on a column, according to a combination of molecular mass and polarity, and sequentially enter the MS source via a heated transfer region. The analytical data consists of total ion chromatograms (TIC) and the mass spectra of the separated components.

Key equations for chromatography

Plate height $H = \frac{L}{N}$

Plate number $N = 5.545 \left(\frac{t_R}{w_{½}}\right)^2$

Adjustment retention time $t'_R = t_R - t_M$

Retention factor $k = \frac{t'_R}{t_M}$

Van Deemter Equation
Capillary (open tubular) GC Column $H = A + \frac{B}{\bar{u}} + C\bar{u}$

Golay equation
Packed GC column $H = A + \frac{B}{\bar{u}} + Cs\bar{u} + C_m\bar{u}$

Resolution $R = \frac{t_{R2} - tR_1}{(W_{b1_+} W_{b2})^2}$

Separation factor $\alpha = \frac{t'_{R2}}{t_{R1}} = \frac{k_2}{k_1}$

Resolution $R_s = \frac{1}{4}\sqrt{N}\left(\frac{a-1}{a}\right)\left(\frac{k_2}{k_{ave}+1}\right)$

In 1901 Mikhail Tswett invented adsorption chromatography during his research on plant pigment. He separated different coloured chlorophyll and carotenoid pigments of leaves by passing an extract of the leaves through a column of calcium carbonate, alumina and sucrose eluting them with petroleum ether/ethanol mixtures. He coined the term chromatography in a 1906 publication, from the Greek words *chroma* meaning "colour" and *graphos* meaning "to write".

The international Union of Pure and Applied Chemistry (IUPAC) has drafted a recommended definition of chromatography:-

"**Chromatography** is a physical method of separation in which the components to be separated are distributed between two phases, one of which is stationary (stationary phase), while the other (the mobile phase) moves in a definite direction". [L.S. Ettre, "Nomenclature for Chromatography", *Pure & Appl. Chem*., 65 (1993), 819-872].

The two principal types of chromatography are gas chromatography (**GC**) and liquid chromatography (**LC**). Gas chromatography separates gaseous substances based on partitioning in a stationary phase from a gas phase. Liquid chromatography includes techniques such as size exclusion (separation based on molecular size), ion exchange (separation based on charge) and high-performance liquid chromatography (HPLC separation based on partitioning from a liquid phase)

Principles of chromatographic separations

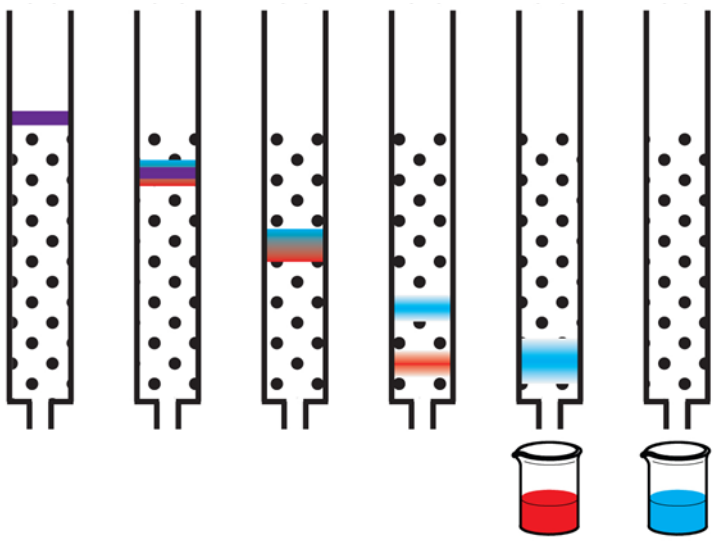
While the mechanisms of retention for various types of chromatography differ, they are all based on the dynamic distribution of an analyte between a fixed stationary phase and a flowing mobile phase. Each analyte will have a certain affinity for each phase.

$$K = \frac{c_s}{c_m}$$

where c_s and c_m are the stationary and the mobile phases concentrations.

The distribution of the analyte between two phases is governed by:- temperature, the physico-chemical properties of compound, the stationary and mobile phases.

Analytes with a large K value will be retained more strongly by the stationary phase than those with a small K value. The result is that the latter will move along the column (be ELUTED) more rapidly.



Classification of chromatographic techniques

Chromatographic processes can be classified according to the type of equilibration process involved, which is governed by the type of the stationary phase.

Various bases of equilibration are:-

1. Adsorption
2. Partition
3. Ion exchange
4. Size dependent pore penetration
5. Gas chromatography

More often that not, analyte stationary-phase-mobile-phase interactions are governed by a combination of such processes.

Adsorption chromatography

The stationary phase is a solid on which the sample components are adsorbed. The mobile phase may be a liquid (*liquid-solid chromatography*) or gas (*gas-solid chromatography*); the components distribute between two phases through a combination of sorption and desorption processes.

Thin-layer chromatography (TLC)

- the stationary phase is planar, in the form of a solid supported on an inert plate, and the mobile phase is a liquid.

Partition chromatography

The stationary phase is usually a liquid supported on a solid or a network of molecules, which functions as a liquid, bonded on the solid support. The mobile phase may be a liquid (*liquid-liquid partition chromatography*) or a gas (*gas-liquid chromatography, GLC*).

Normal phase chromatography has a polar stationary phase (*e.g.* cyano groups bonded on silica gel) and the mobile phase is non-polar (*e.g.* hexane). When analytes dissolved in the mobile phase are introduced into the system, retention increases with increasing polarity.

Reversed phase chromatography has a non-polar stationary phase and a polar mobile phase, the retention of analytes decreases with increasing polarity.

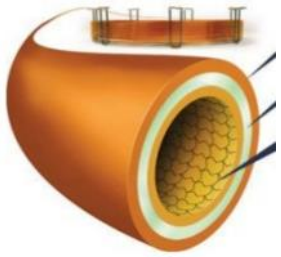
Gas chromatography (GC)

There are two types of GC :-

- Gas-solid (adsorption) chromatography
- Gas-liquid (partition) chromatography

In every case, successive equilibria determine to what extent the analyte stays behind in the stationary phase (adsorption chromatography) or are coated with a thin layer of liquid phase (partition chromatography).

Most common form today is a capillary column, in which a virtual liquid phase, often polymer, is coated or bonded on the wall of the capillary tube.



Special high temperature polyimide coating

Fused silica

Stationary phase with Engineered Self Cross-linking (ESC) technology

Theory of column efficiency in chromatography

Band broadening in chromatography is the result of several factors, which influence the efficiency of separations. The separation efficiency of a column can be expressed in terms of the number of theoretical plates in the column.

$$H = \frac{L}{N}$$

H - the plate height (has dimensions of length, μm)

L - the column length

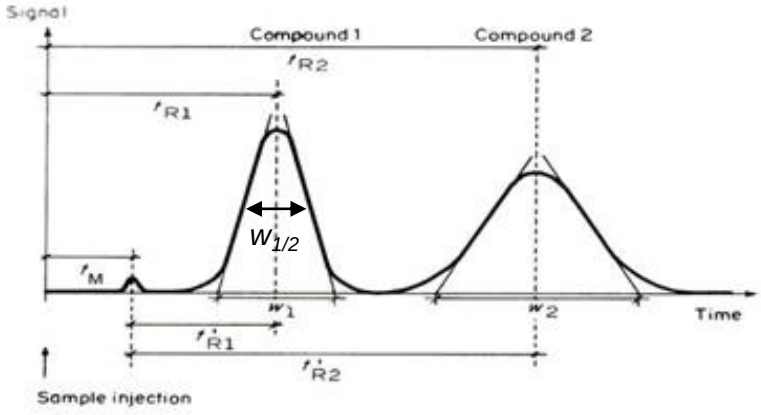
N - the number of theoretical plates

The more the number of plates, the more efficient is the column.

Experimentally, the plate height is a function of the variance, σ^2, of the chromatographic band and the distance, x, it has travelled through the column, and is σ^2/x; σ is the standard deviation of the Gaussian chromatographic peak.

The width at half-height, $w_{1/2}$, corresponds to 2.355σ, and the base width w_1 corresponds to 4σ. The number of plates, N, for an analyte eluting from a column:-

$$N = \left(\frac{t_R}{\sigma}\right)^2$$



Putting in $w_{1/2}$ =2.355σ then N= $5.545(\frac{t_R}{W_{1/2}})^2$

(N, the number of plates of a column, is strictly applicable for that specific analyte, t_R is the retention time, $w_{1/2}$ is the peak width at half-height in the same units as t_R)

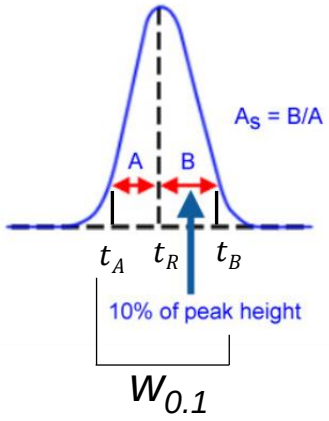
N = $16(\frac{t_R}{W_b})^2$

The *effective plate number* corrects theoretical plates for dead volume and hence is a measure of the true number of useful plates in a column:

N_{eff} = $5.545(\frac{t'_R}{W_{1/2}})^2$

t'_R is the adjusted retention time $t'_R = t_R - t_M$

t_M is the time required for the mobile phase to traverse the column and is the time it would take for an unretained analyte to appear.



For asymmetric peaks, the efficiency is determined by the Foley-Dorsey equation.

$N_{sys} = \frac{41.7\left(\frac{t_R}{w_{0.1}}\right)^2}{\frac{B}{A}+1.25}$

A+B = $w_{0.1}$ are the widths from t_R to the left and right sides

Once N is known, H can be obtained or H_{eff} =L/N_{eff} and normally determined for the last eluting compound.

Rate theory of chromatography - the Van Deemter equation

The retention factor, *k* is the ratio of the time the analyte spends in the stationary phase to the time it spends in the mobile phase.

$k = \frac{t'_R}{t_M}$

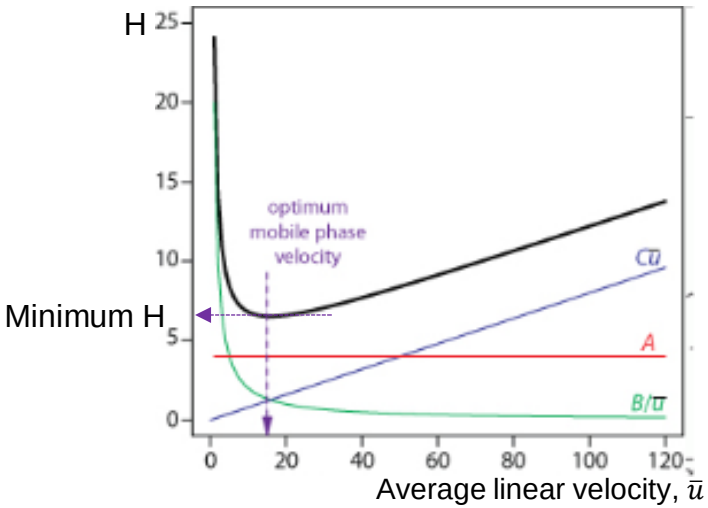
$H = A + \frac{B}{\bar{u}} + C\,\bar{u}$ *For a packed GC column the van Deemter equation*

A, B and *C* are constants for a given system and related to the three major factors affecting H, and $\bar{u}$ is the average linear velocity of the carrier gas in cm/s.

$\bar{u} = L/t_M$

t_M is the time for an unretained substance to elute

The general flow term for chromatography is the mobile-phase velocity, *u*. However, in GC, the linear velocity will be different at different positions along the column due to the compressibility of gases. The average linear velocity $\bar{u}$ is used.



The significance of the three terms, A, B and C in packed column GC is shown as a plot of H as a function of carrier gas velocity.

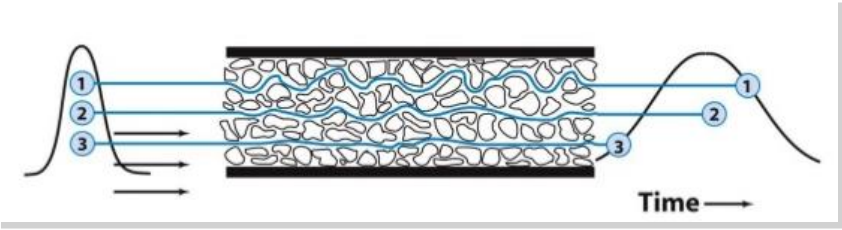
A- Eddy diffusion and is due to the variety of variable length pathways available between the particles in the column and is independent of the gas- and mobile-phase velocity and relates to the particle size and geometry of packing.

$A = 2\lambda d_p$

λ- an empirical constant

(depend how well the column is packed)

d_p -the average particle diameter

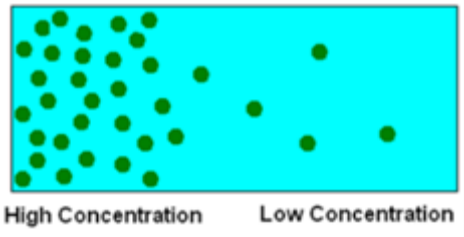


B - Longitudinal (axial) or molecular diffusion of the sample components in the carrier gas, due to concentration gradients within the column.

$B = 2\gamma D_m$

ɣ- an obstruction factor, typically equal to 0.6 to 0.8 in a packed GC column

D_m -the diffusion coefficient



Molecular diffusion

Molecular diffusion is a function of both the sample and the carrier gas. The sample components are fixed, and to change B or $B/\bar{u}$ is by varying the flow rate of the carrier gas. High flow rates reduce the contribution of molecular diffusion and the total analysis time.

C – the interphase mass transfer term and is due to the finite time required for solute distribution equilibrium to be established between the two phases as it moves between the mobile and stationary phases. The *C*-term has two separate components, C_m and C_s, respectively, representing mass transfer limitations in the mobile and the stationary phases.

The C_m term originates from non-uniform velocities across the column cross section.

$C_m = \frac{C_1 \omega {d_p}^2}{D_m} u$ *for uniformly packed columns*

C_1 – a constant; ω – related to the total volume of mobile phase in the column

The stationary phase mass transfer term, C_s, is proportional to the amount of stationary phase, and increase with the retention factor for the analyte and the thickness of the stationary phase film d_f. $\frac{{d_f}^2}{D_s}$ represents the characteristic time for the analyte to diffuse in and out of the stationary phase.

$C_s = C_2 \frac{k}{(1+k)} \frac{{d_f}^2}{D_s} u$

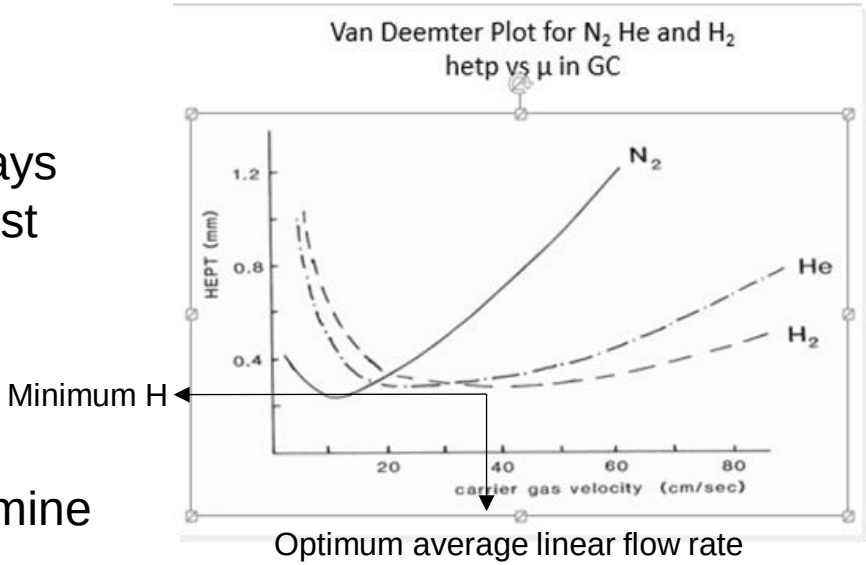
Open tubular column have no packing, A-term in van Deemter equation disappears.

$H = \frac{B}{\bar{u}} + C\,\bar{u}$ *Golay equation*

An efficient packed GC column will have several thousand theoretical plates, and capillary columns have plate counts depending on the column internal diameter 3,800 plates/m for 0.32 mm i.d. column a film thickness of 0.32 µm to 6,700 plates/m for a 0.18 mm i.d column with 0.18 µm film thickness (for an analyte of *k*=5). The GC columns are typically 20-30 m long and total plate counts can be well in excess of 100,000.

GC mobile phase

The mobile phase (carrier gas) is almost always helium, nitrogen or hydrogen, with helium most popular.
Gases should be pure and chemically inert.
Impurities level should be less 10 ppm.



Flow rate is one of the parameters that determine the choice of carrier gas via the van Deemter plot, the minima in these plots, defined as the optimum values of *u.*

Hydrogen provides the highest value of u_{opt} of three common carrier gases, resulting in the shortest analysis time. The van Deemter curve is very flat, which provides a wide range over which high efficiency is obtained.

Retention factor efficiency and resolution

The retention factor *k*

$k = \frac{t'_R}{t_M}$ is a direct measure of how strongly an analyte is retained by the column under the given conditions.

If a pair of analytes are poorly separated, separation improves if chromatographic conditions (temperature in GC, eluent strength in LC) are altered to increase *k*.

While a large retention factor favours good separation, large retention factors mean increased elution time, so there is a compromise between separation efficiency and separation time. The retention factor could be increased by increasing the stationary phase volume.

The effective plate number is related to the retention factor and plate number via:-

$N_{eff} = N \left(\frac{k}{k+1}\right)^2$

Resolution in chromatography

The resolution of two chromatographic peaks:-

$R_s = (t_{R2} - tR_1)/[(wb_1 + wb_2)/2]$

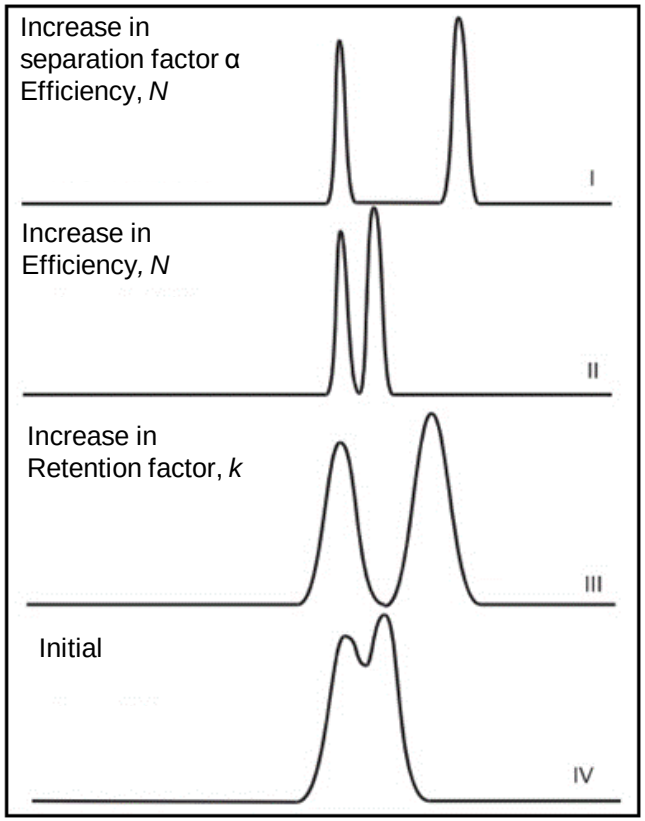
t_{R1} and t_{R2} are the retention times of the two peaks (peak 1 elutes first)

w_{b1} is the baseline width of the peaks.

The separation factor, α, also the selectivity and is a thermodynamic quantity that is a measure of the relative retention of analytes.

$$\alpha = \frac{t'_{R2}}{t_{R1}} = \frac{k_2}{k_1}$$

k_2 and k_1 are the retention factors of the adjusted retention times. This describes how well the chromatographic conditions discriminate between the two analytes.



$$R_s = \frac{1}{4}\sqrt{N}\left(\frac{a-1}{a}\right)\left(\frac{k_2}{k_{ave}+1}\right)$$

k_{ave} is the mean of the two capacity factors.

N is proportional to L, the R_s is proportional to $\sqrt{L}$. So doubling the column increases the R_s by $\sqrt{2}$ or 1.4. The retention times would be increased in direct proportion to the length of the column.

Gas chromatography columns

The two types of columns are:-

- Packed columns
- Capillary columns

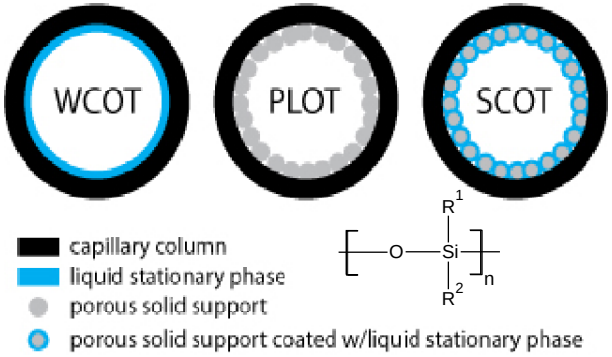
Packed columns can be in any shape, 1 to 10 m long and 0.2 to 0.6 cm in diameter. They made of stainless steel, nicker or Teflon. Long columns require high pressure and longer analysis time. The column is packed with small particles that may themselves serve as the stationary phase (adsorption chromatography) or more commonly are coated with a non-volatile liquid phase or varying polarity (partition chromatography).

Gas solid chromatography (GSC) is for separation of small gaseous species such as H_2, N_2, CO_2, CO, O_2, NH_3 and CH_4 and volatile hydrocarbons, using high surface area inorganic packings such as alumina or porous polymer. The gases are separated by their size due to retention by adsorption on the particles.

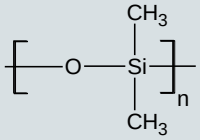
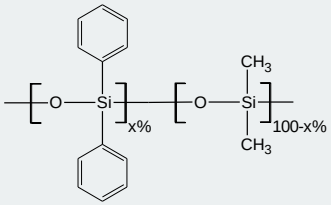
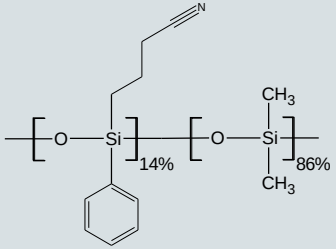
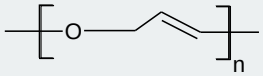
The solid support for a liquid phase have a high specific surface area, chemically inert, thermally stable and have uniform sizes. The most common used supports are prepared from diatomaceous earth, a spongy siliceous material. Particles have diameters in the range of 60 to 80 mesh (0.18 to 0.25 mm), 80 to 100 mesh (0.15 to 0.18 mm) or 100 to 120 mesh (0.12 to 0.15 mm)

Capillary columns – the most widely used

A narrow open tubular columns with the stationary phase supported on the inner wall shows increase number of plates, band broadening due to multiple paths is eliminated and rate of mass transfer is increased since molecules have small distance to diffuse. Higher flow rate can be used due to decreased pressure drop. These columns are made of thin (SiO_2) coated on the outside with a polyimide polymer for support. The inner surface of the capillary is chemically treated by reacting the Si-OH group with a silane-type reagent.
The capillaries are 0.10 to 0.53 mm internal diameter, with lengths of 15 to 100 m can have several hundred thousand plates.

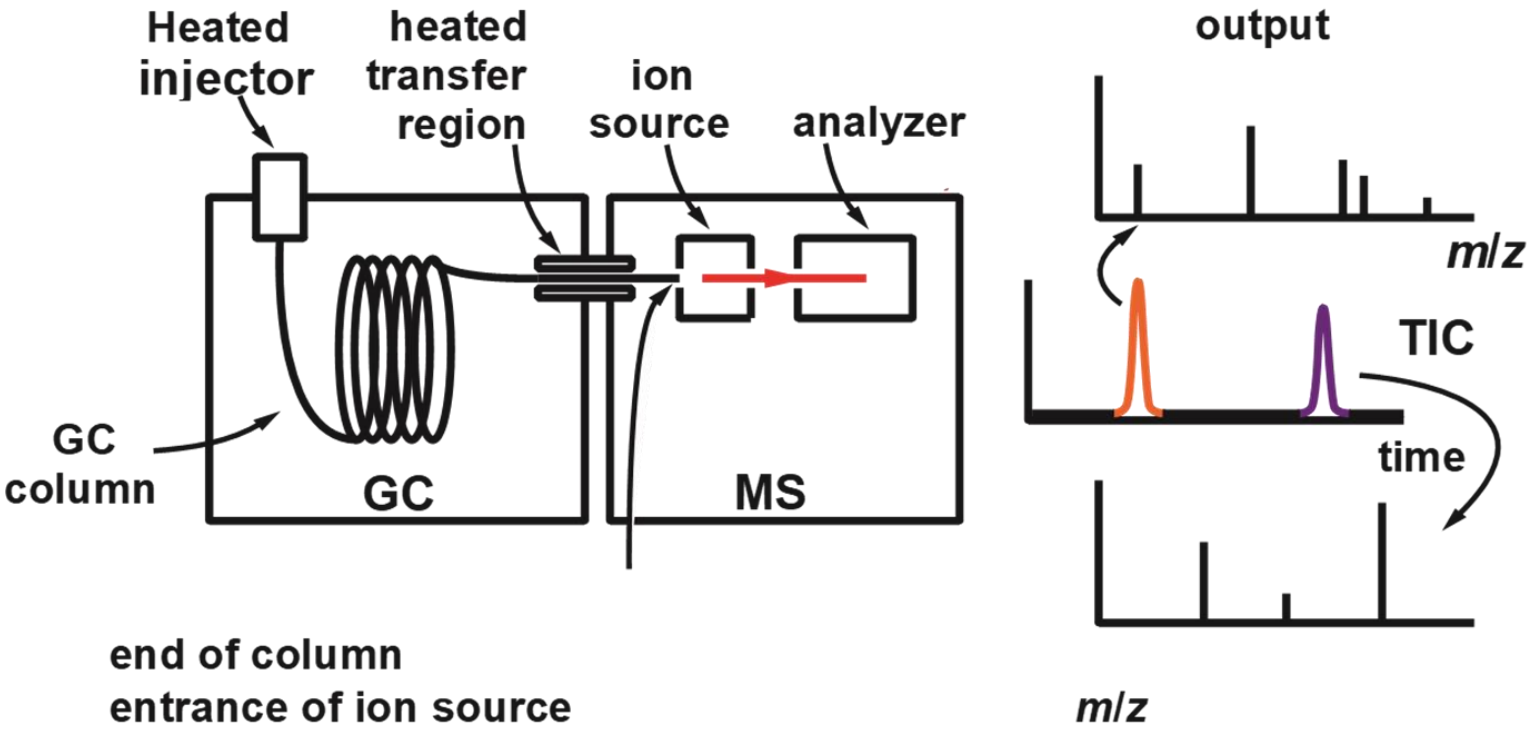


There are three types of open-tubular columns:-
Wall coated open tubular (WCOT) have a thin liquid film coated on and supported by the walls of the capillary. The stationary phase is 01. to 0.5 µm thick.
In support coated open-tubular (SCOT) columns, solid microparticles coated with the stationary phase (much like in packed column) and attached to the walls of the capillary.
Porous layer open tubular (PLOT) columns, have solid-phase particles attached to the column wall, for adsorption chromatography. Particles alumina or porous polymers are used.

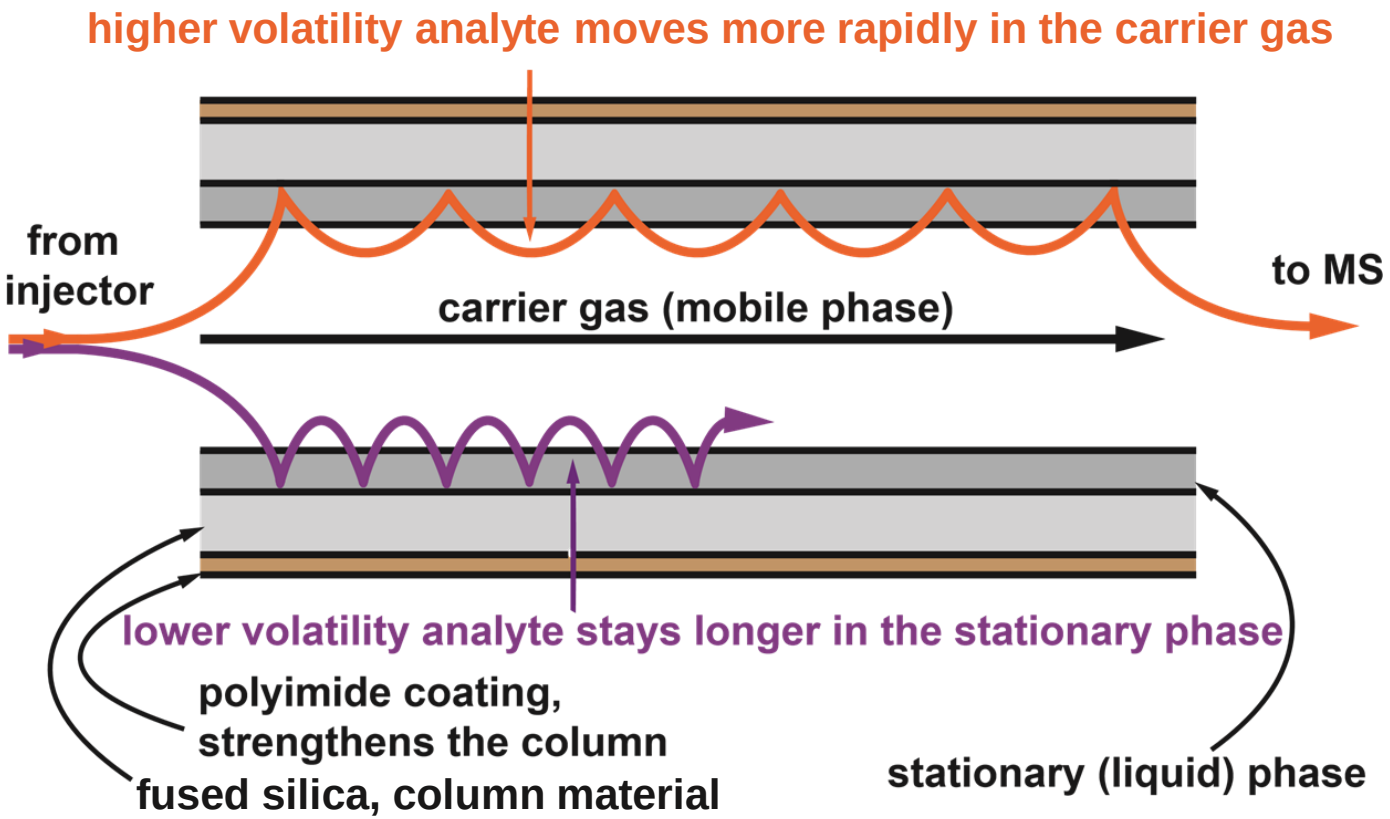
Phase	Polarity	Use	Max Temp. (°C)
100% dimethyl polysiloxane 	Nonpolar	Basic general purpose phase for routine use. Hydrocarbons, polynuclear aromatics, PCBs	320
Diphenyl, dimethyl polysiloxane 	Low (x=5%) Intermediate (x=35%) Intermediate (x=65%)	General purpose, good high temperature characteristics. Pesticides.	320 300 370
14% cyanopropylphenyl-86%dimethylsiloxane 	Intermediate	Separation of organochlorine pesticides listed in EPA 608	280
Poly(ethyleneglycol) Carbowax 	Very polar	Alcohols, aldehydes, ketones and separation of aromatic isomers	250

Phases are selected based on their polarity, keeping in mind that “like dissolve like”. A polar stationary phase will interact more with polar compounds and vice versa. Non-polar liquid phase are nonselective so separations tend to follow the order of the boiling points of analytes. Polar liquid phases exhibit several interactions with analytes such as dipole interactions, hydrogen bonding, and induction forces, there is often no correlation between the retention factor or volatility.

Gas chromatography mass spectrometry (GC-MS)



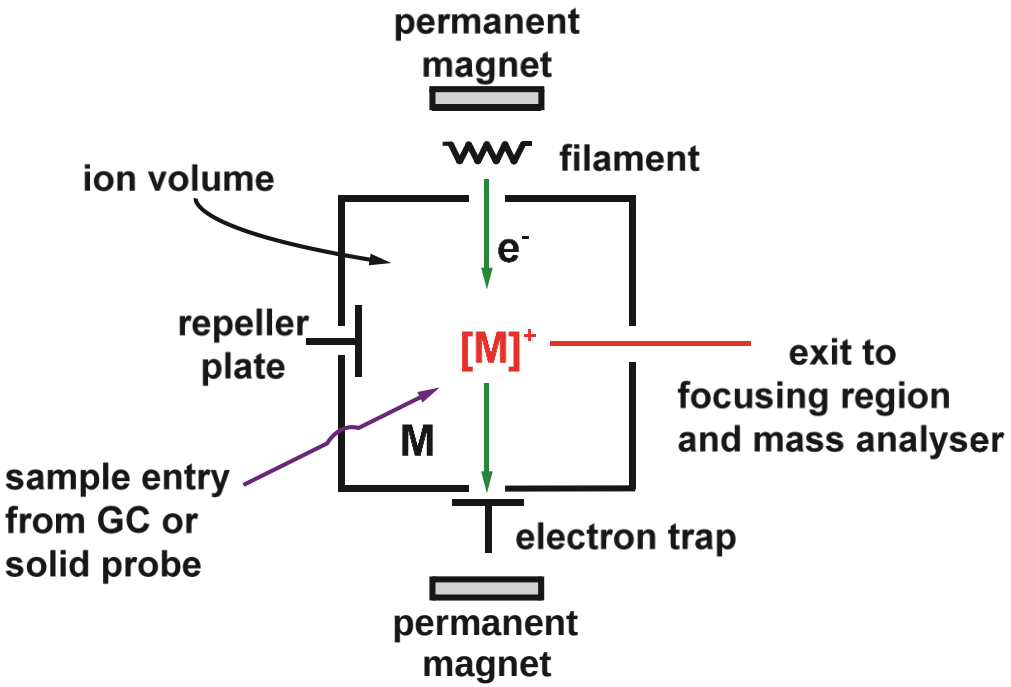
Samples are introduced into the GC using a heated injector. Components are separated on a column, according to a combination of molecular mass and polarity, and sequentially enter the MS source via a heated transfer region. The analytical data consists of total ion chromatograms (TIC) and the mass spectra of the separated components.



Analytes condense at the entrance of the column and are subsequently separated based on their molecular mass and polarity. These properties determine analyte volatility and, as a result, the retention times in the stationary liquid phase and the gaseous mobile phase. More volatile components elute first as they are carried through the column by the carrier gas at lower temperatures. Increasing the oven temperature enables the transfer of compounds with higher boiling points from the stationary phase into the vapour phase and their elution from the column.

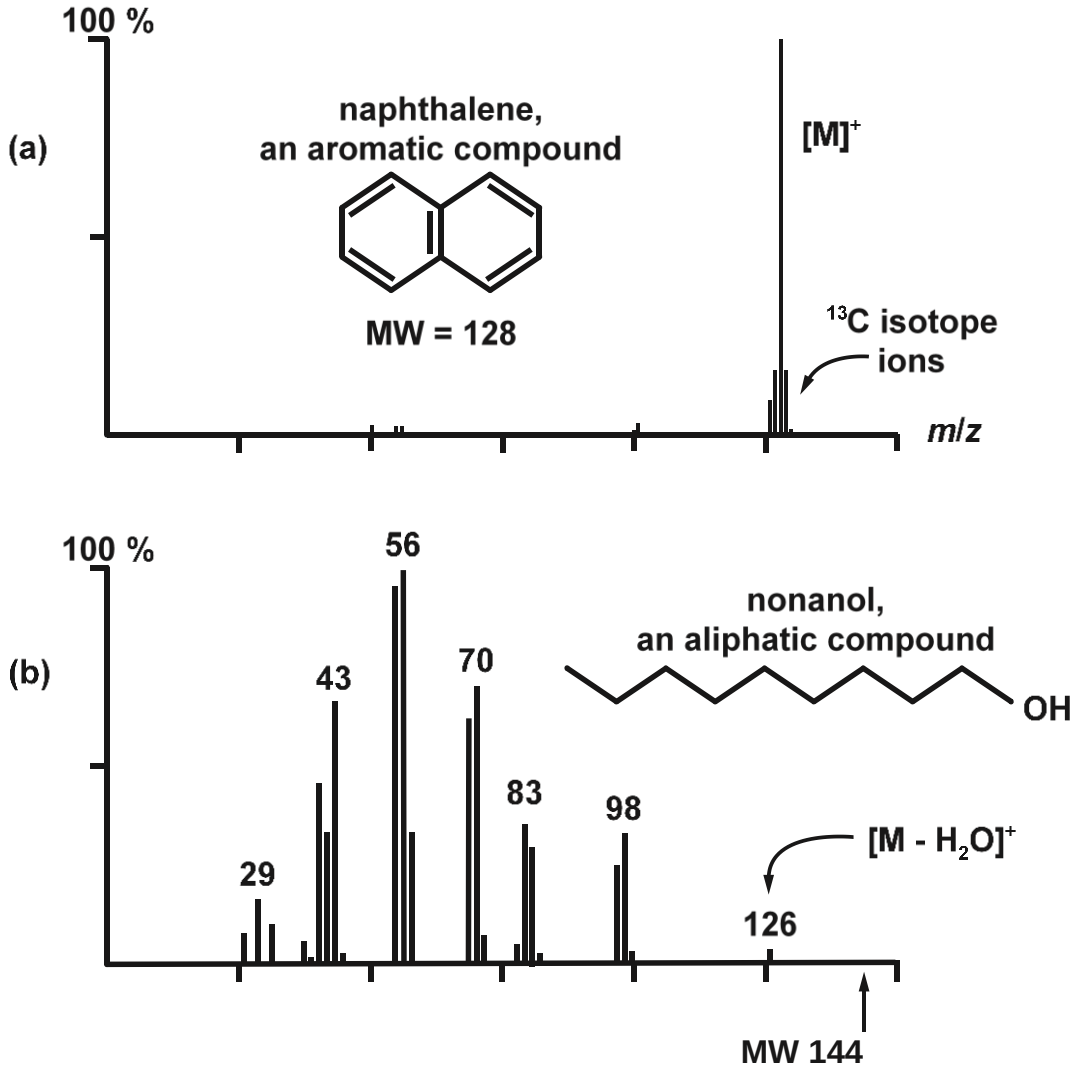
Ionisation methods – Electron Impact Ionisation (EI)

- Sample molecules are vaporised and introduced into the EI source (the analysis of gases or small volatile molecules)
- Derivatisation is required for the analysis of non-volatile thermally-labile compounds
- Electrons are generated by thermionic emission from a hot filament, just like a light bulb
- The electrons are accelerated into the region containing gaseous sample called the “source block”.



- An electron energy of 70 eV is commonly used in EI
- Energetic electrons can ionise molecules
  $e^- + M \rightarrow M^{+\bullet} + 2e^-$
- At 70 eV, the molecular ion ($M^{+\bullet}$) formed may fragment.
- Ions are accelerated out of the ion source and transmitted the mass analyser to the detector.

Comparison of the EI spectra for (a) an aromatic and (b) an aliphatic compound

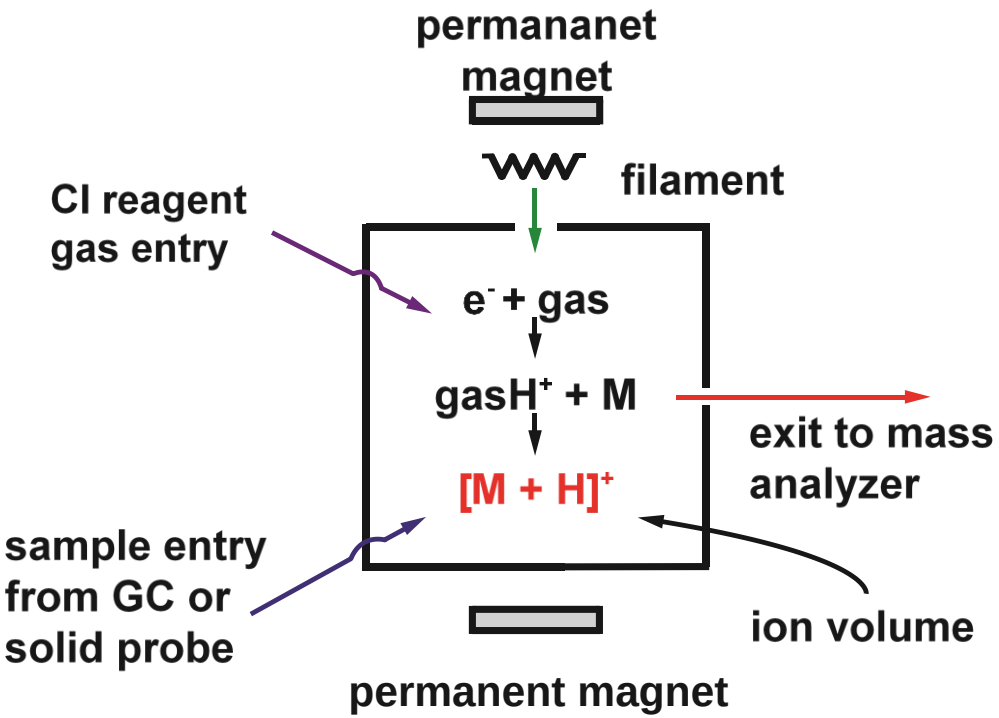


Libraries (EI).

i. Over the past forty-fifty years, since mass spectrometry has become a standard tool, libraries of mass spectra have been generated.

ii. The newest libraries contain hundreds of thousands of EI mass spectra from which an unknown compound can very often be identified.

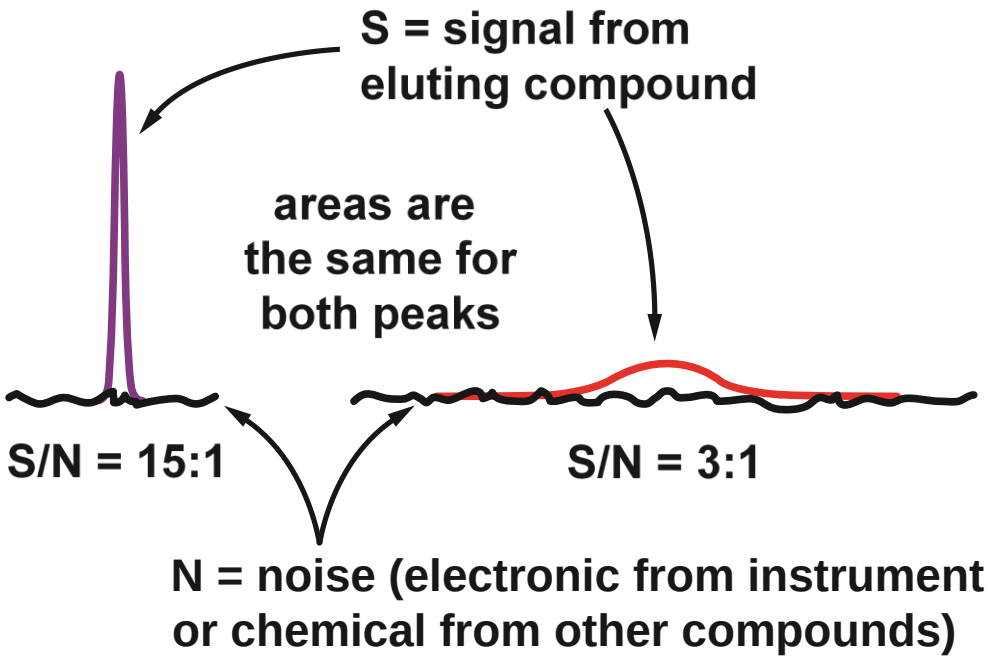
Chemical ionisation (CI) source



Electrons from the filament react with a reagent gas (methane, isobutane or ammonia) generating protonated reagent species that transfer a proton onto, or form an adduct with, the analyte.

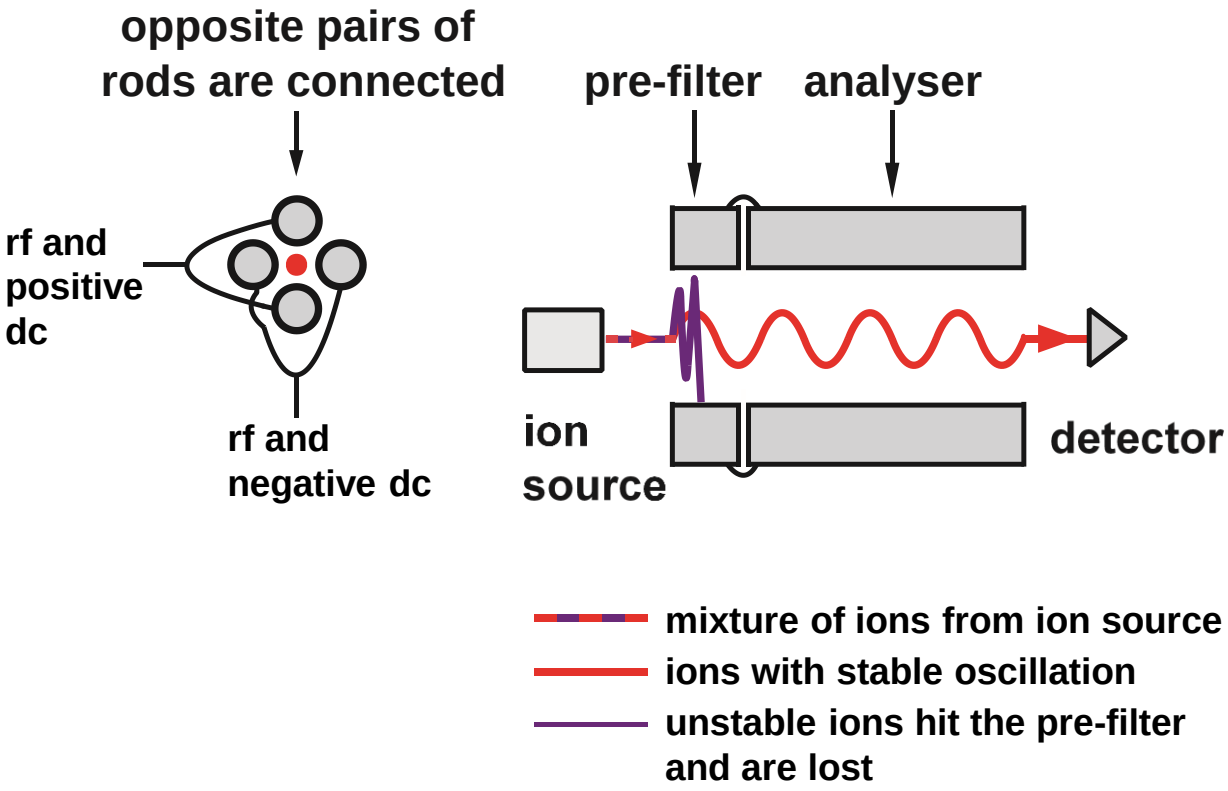
e.g., $M + [NH_4]^+ \rightarrow [M + H]^{+\cdot}$ and/or $[M + NH_4]^{+\cdot}$

Signal-to-noise ratio vs. peak width



The signal-to-noise (S/N) ratio improves when the width of the chromatographic peak is reduced. The amount of material injected is the same in both cases shown. However, the number of ions arriving per unit time at the detector, i.e., the concentration, increases as the peak narrows. The higher concentration improves the S/N ratio. In the illustration the detection limit is increased by a factor of five.

Quadrupole (Q) analyser



For any given set of rf and dc voltages, on the opposing pairs of rods, only ions of one *m*/*z* ratio display a stable oscillation enabling them to reach the detector. Unstable ions hit the initial part of the analyser, often a pre-filter, are discharged and lost. The pre-filter, which is connected electrically to the analyser, is not essential, but can be removed conveniently for cleaning.

Mass of the elements.

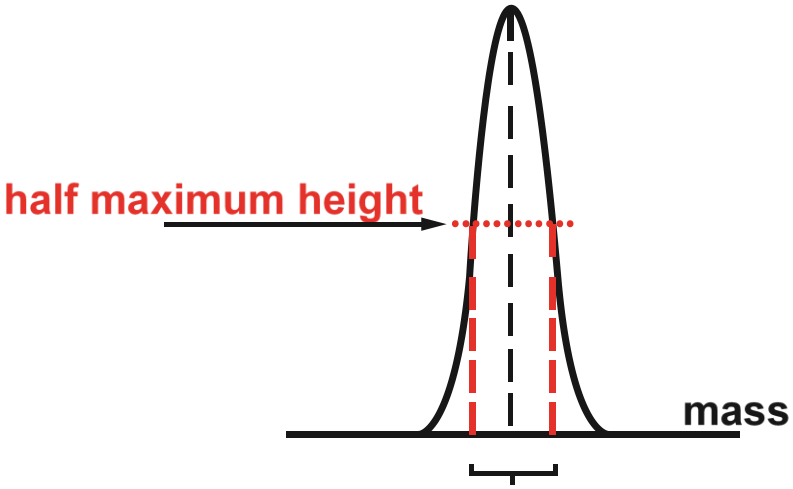
1. Today carbon **^{12}C** is taken to have an atomic mass of **12.000000000 Da.**
2. The atomics masses of the other elements and their isotopes are measured relative to this.
3. The relative atomic masses of some elements are listed below:-
   ^{12}C =12.00000000
   ^{1}H = 1.007825035
   ^{14}N =14.003074002
   ^{16}O =15.99491463
4. The molecular mass of ammonia (NH3) =14.003074002+(3x1.007825035) =17.026549
   The molecular mass of OH = 15.99491463+1.007825035 =17.00274
5. By **accurately measuring** the molecular mass of a sample its **elemental composition** can be determined.

Monoisotopic mass- the mass of an ion which is made up of the lightest stable isotopes of each element (includes the mass defect, where ^{1}H=1.0078, ^{12}C=12.0000, ^{16}O=15.9949 etc).

Average mass- the mass of an ion calculated using the relative average isotopic mass of each element (where, C=12.0111, H=1.00797, O=15.9994 etc).

Isotopic Abundance- the naturally occurring distribution of the same element with different atomic mass e.g. ^{12}C=12.0000=98.9%,^{13}C=13.0034=1.1%

The resolution of one mass from another and the sensitivity of ion detection are arguably the most important performance parameters of a mass spectrometer.



$$\text{Resolution} = \frac{\text{mass}}{\text{width at half maximum height}}$$

Resolution is a measure of the ability of a mass analyser to separate ions with different *m/z* values.

Resolution determined experimentally from the measured width of a single peak at a defined percentage height of that peak and then calculated as $m/\Delta m$, where m equals mass and Δm is the width of the peak.

The full width of the peak at half its maximum height (FWHM) is the definition of resolution used most commonly.