pH

It expresses the intensity of the acid or the alkaline condition of a solution. It also expresses the hydrogen ion concentration or the hydrogen-ion activity.
The acids contain the element hydrogen whereas bases contain hydroxyl group.
It is expressed as the log of the reciprocal of the hydrogen ion concentration.
i.e $pH = \log \frac{1}{[H^+]}$. The scale of pH varies from 0-14. For neutral waters (i.e. in absence of foreign materials, pH = 7. At this stage, the $[H^+] = [OH^-]$. A lower pH value indicates higher hydrogen ion concentration and hence an acidic nature of the solution

$H_2O \rightleftharpoons H^+ + OH^-$. Since water dissociates to produce one hydroxyl ion for each hydrogen ion, then the concentration of $[H^+]$ ions = $[OH^-] = 10^{-7}$ mg/l.
From equilibrium =n, $\frac{[H^+][OH^-]}{[H_2O]} = k$. Since quantity of water is very large, there will not be much change in the concentration of the whole water. Thus $[H_2O]$ can be treated as constant.

$\therefore [H^+][OH^-] = k_w$ (cross multiplying)

For pure water at 25°C, $[H^+][OH^-] = 10^{-7} \times 10^{-7} = 10^{-14} = k_w$. This is called as ion product or ionization constant for water.

When acids are added, the hydrogen ion concentration increases. Likewise, the hydroxyl ion concentration decreases.

i.e. if hydrogen ion concentration = 10^{-1}, $[OH^-] = 10^{-13}$. and vice versa.

Gas chromatography

Gas chromatography (GC) is a common type of **chromatography** used in analytical chemistry for separating and analyzing compounds that can be vaporized without decomposition.

Gas chromatography (**GC**) is a technique **used for** the analysis and quantification of **volatile compounds**. Compounds are injected onto the **gas chromatograph** and flash evaporated onto the column. This can be done using a packed or capillary column. The column is the stationary phase and the **gas** is the mobile phase.

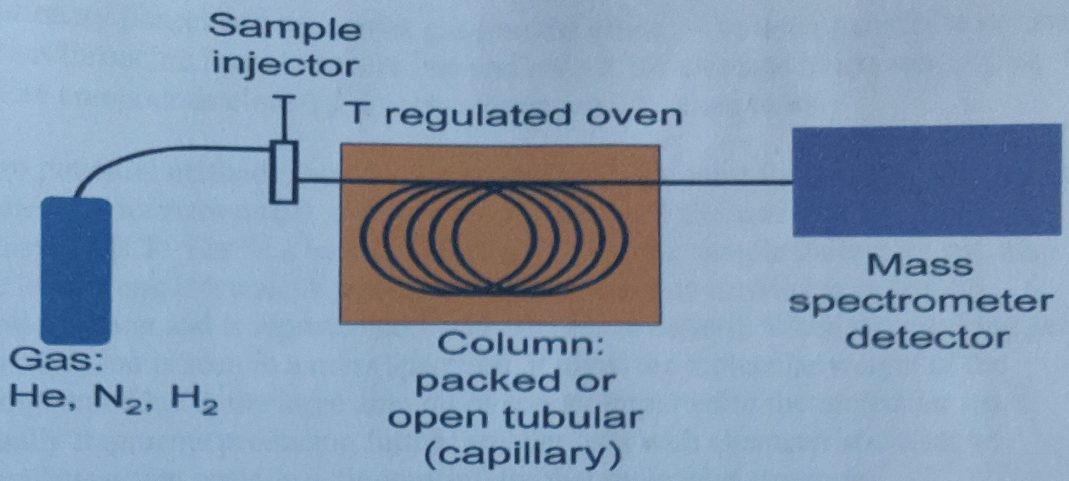
Principle of **gas chromatography**: The sample solution injected into the instrument enters a **gas** stream which transports the sample into a separation tube known as the "column." (Helium or nitrogen is used as the so-called carrier **gas**.) The various components are separated inside the column .To separate the compounds in **gas**-liquid **chromatography**, a solution sample that contains organic compounds of interest is injected into the sample port where it will be vaporized. The vaporized samples that are injected are then carried by an inert **gas**, which is often used by helium or nitrogen.

Applications of GC-MS include drug detection, fire investigation, environmental analysis, explosives investigation, and identification of unknown samples.

WORKING

The GC-MS is composed of two major building blocks: the gas chromatograph and the mass spectrometer. The gas chromatograph utilizes a capillary column which depends on the column's dimensions (length, diameter, film thickness) as well as the phase properties (e.g. 5% phenyl polysiloxane). The difference in the chemical properties between different molecules in a mixture and their relative affinity for the stationary phase of the column will promote separation of the molecules as the sample travels the length of the column. The molecules are retained by the column and then elute (come off) from the column at different times (called the retention time), and this allows the mass spectrometer downstream to capture, ionize, accelerate, deflect, and detect the ionized molecules separately. The mass spectrometer does this by breaking each molecule into ionized fragments and detecting these fragments using their mass-to-charge ratio.

Add equations



These two components, used together, allow a much finer degree of substance identification than either unit used separately. It is not possible to make an accurate identification of a particular molecule by gas chromatography or mass spectrometry alone. The mass spectrometry process normally requires a very pure sample while gas chromatography using a traditional detector (e.g. Flame ionization detector) cannot differentiate between multiple molecules that happen to take the same amount of time to travel through the column (*i.e.* have the same retention time), which results in two or more molecules that co-elute.

Sometimes two different molecules can also have a similar pattern of ionized fragments in a mass spectrometer (mass spectrum). Combining the two processes reduces the possibility of error, as it is extremely unlikely that two different molecules will behave in the same way in both a gas chromatograph and a mass spectrometer. Therefore, when an identifying mass spectrum appears at a characteristic retention time in a GC-MS analysis, it typically increases certainty that the analyte of interest is in the sample.

WORKING:

The sample solution is injected into the GC inlet where it is vaporized and swept onto a chromatographic column by the carrier gas (usually helium). The sample flows through the column and the compounds comprising the mixture of interest are separated by virtue of their relative interaction with the coating of the column

(stationary phase) and the carrier gas (mobile phase). The latter part of the column passes through a heated transfer line and ends at the entrance to ion source (Fig. 1) where compounds eluting from the column are converted to ions.

Two potential methods exist for ion production. The most frequently used method is electron ionisation (EI) and the occasionally used alternative is chemical ionisation (CI). For EI a beam of electrons ionise the sample molecules resulting in the loss of one electron. A molecule with one electron missing is called the molecular ion and is represented by $M^{+\cdot}$ (a radical cation). When the resulting peak from this ion is seen in a mass spectrum, it gives the molecular weight of the compound. Due to the large amount of energy imparted to the molecular ion it usually fragments producing further smaller ions with characteristic relative abundances that provide a 'fingerprint' for that molecular structure.

This information may be then used to identify compounds of interest and help elucidate the structure of unknown components of mixtures. CI begins with the ionisation of methane (or another suitable gas), creating a radical which in turn will ionise the sample molecule to produce $[M+H]^+$ molecular ions. CI is a less energetic way of ionising a molecule hence less fragmentation occurs with CI than with EI, hence CI yields less information about the detailed structure of the molecule, but does yield the molecular ion; sometimes the molecular ion cannot be detected using EI, hence the two methods complement one another. Once ionised a small positive is used to repel the ions out of the ionisation chamber.

The next component is a mass analyser (filter), which separates the positively charged ions according to various mass related properties depending upon the analyser used. Several types of analyser exist: quadrupoles (Fig. 2), ion traps, magnetic sector, time-of-flight, radio frequency, cyclotron resonance and focusing to name a few. The most common are quadrupoles and ion traps. After the ions are separated they enter a detector the output from which is amplified to boost the signal. The detector sends information to a computer that records all of the data produced, converts the electrical impulses into visual displays and hard copy displays. In addtion, the computer also controls the operation of the mass spectrometer