ASSIGNMENT No. 1

Q. 1 Point out and discuss the summer fiel's modification of Azimuthal Quantum Number.

The **quantum numbers** are basically represents the address of an electrons in atom. These quantum numbers represent the location, energy level and spin of electron in atom. These quantum numbers are useful for representing the electron configuration. **Quantum numbers** are of four types –

1. Principal quantum number (n)
2. Orbital or Azimuthal quantum number (l)
3. Magnetic quantum number (m or m_l)
4. Spin magnetic quantum number (m_s)

Principal Quantum Number (n)

Principal quantum number of an electron represents the main energy level or shell or orbit to which the electron belongs. It is represented by 'n'. It has integral values i.e. 1, 2, 3, 4, ……etc. Principal quantum number is used in Bohr and Summer field atomic model. The electrons having principal quantum number, are associated with same energy levels (shells). These energy levels are denoted by the letters K, L, M, N, ……. etc. For different energy level (shells) the value of "Principal quantum Number 'n' and maximum number of electrons associate with different energy levels are given in table below-

Sl. No.	Energy level or Orbit (shell)	Principal quantum number 'n'	Maximum Number of electrons ($2n^2$)
1	K	1	$2 \times 1^2 = 2$
2	L	2	$2 \times 2^2 = 8$
3	M	3	$2 \times 3^2 = 18$
4	N	4	$2 \times 4^2 = 32$

As the **quantum number** of a shell increase the distance of shell increase. Therefore, the shells are having different energy levels which decreases with increase of quantum number.

Orbital or Azimuth Quantum Number (l)

Orbital or azimuth quantum number represents the subshell of orbital to which the electron is associated. The each main shell (energy level) is subdivided into sub energy levels/subshells.

These subshell are also called orbitals. These subshell /orbitals are designated by s, p, d, f, ……. etc. with corresponding orbital quantum number l = 1, 2, 3, 4……etc. The number subshells is any main shell is equal to principal quantum number 'n'. The capacity of any main shell can be determined by adding the electron capacity of subshells. The capacity of subshells are given in table below-

Sl. No.	Subshell	Quantum number (l)	Electron capacity of subshell $2(2l + 1)$
1	s	1	$2(2 \times 0 + 1) = 2$
2	p	2	$2(2 \times 1 + 1) = 6$
3	d	3	$2(2 \times 2 + 1) = 10$

| 4 | f | 4 | | $2(2 \times 3 + 1)=14$ |

The orbital or azimuth **quantum number** represents the angular momentum and possible shape of orbital to which the electron is associated. For Example: for orbital quantum number, $l = 0$, the value of angular momentum is zero and shape of orbital is straight line with zero angular momentum is. For $l = 1$, shape of orbital is an ellipse with some non-zero value of angular momentum. For $l = 2$, shape of orbital is rounder ellipse with more value of angular momentum. For different values of orbital or azimuth quantum number, the shape of orbitals is shown in table below- In electron configuration, the principal **quantum number** is stated just before the letter and the number of electrons with same orbital quantum number is represented as superscript of letter. For example: If an atom is having 6 electrons with principal quantum number 2 in subshell of 'p'. Then in electron configuration it will be denoted as'$2p^6$'.

Magnetic Quantum Number (m or m_l)

The magnetic quantum number (m_l) represents the orbitals of a given subshell. For a given value of l, the value of magnetic **quantum number** (m_l) ranges form $-l$ to $+l$. For example, for p-subshell, the value of m_l will be, $m_l = -1, 0, +1$. The orbitals are represented as p_x, p_y and p_z. Where, the subscript represents the direction of axis of rotation. For given value of l, there are $2l + 1$ possible values of m_l. The shell with principal quantum number of 'n', has n^2 orbitals in that shell (energy level). For subshells the number of possible orbitals and magnetic **quantum numbers** are given in table below-

Subshell	Orbital or Azimuthal quantum number (l)	Number of Orbital $3l + 1$	Magnetic quantum number (m or m_l)
s	0	1	0
p	1	$3(p_x, p_y, p_z)$	$-1, 0, +1$
d	2	$5 (d_x^2\text{-}y^2, d_z^2, d_{xy}, d_{xz}, d_{yz})$	$-2, -1, 0, +1, +2$
f	3	$7(f_z^3, f_{xz}^2, f_{xyz}, f_{x(x}^2\text{-}3y^2), f_{yz}^2, f_{z(x}^2\text{-}y^2), f_{y(3x}^2\text{-}y^2))$	$-3, -2, -1, 0, +1, +2, +3$

Spin Magnetic Quantum Number (m_s)

As the earth revolve around the sun and rotates about it axis, in similar way the electrons in atom revolves around nucleus and rotates about its axis which is called 'Spin' of electron. The direction of rotation (spin) of electrons about it axis is represented by "Spin magnetic quantum number". This **quantum number** does not affects the energy level of electrons. The "Spin magnetic quantum number"can only have one value either $+ 1/2$ or $- 1/2$. In general, the electron with $m_s = + 1/2$ is called an alpha electron, and electron with $m_s = - 1/2$, is called beta electron. No two paired electrons can have same spin value.

Q. 2 Describe the Le Chatelier's Principle and its industrial applications.

Chemical equilibrium is a state in the course of a chemical reaction where the concentrations of both products and reactants reach the limit which prevents further deviation. Le-Chatelier's principle is one of the pivotal ideas to understand the behaviour of a system in equilibrium. It states that "If a dynamic equilibrium is disturbed by changing the conditions, the position of equilibrium moves to partially reverse the change". Another important idea which led to further development on this science, is the usage of Gibb's free energy for quantifying the equilibrium. It is stated as "Equilibrium is attained when the Gibbs free energy of the system is at its minimum value (assuming the reaction is carried out at constant temperature and pressure)". The equilibrium constant for a reaction finds its relation to the Gibb's free energy as:

$$\Delta_r G^\ominus = -RT \ln K_{eq}$$

R is the universal gas constant and T is the temperature.

Le-Chatelier's principle of equilibrium is used in the industrial applications as the reaction scheme involves parameters like temperature, pressure, concentration of reaction species a change in even single parameter results in the change of equilibrium leads to undesired product formation. The optimal parameter maintenance in the reaction scheme helps in achieving the desired product. Since the major product is highly desirable in industrial applications for profitability, unless the system yields the loss is effected due to undesired product. A mistake by operator of the process will result in costly loss to the process industry. The concentration of both reactant and product plays a vital role in equilibrium; for example, if the reactant concentration is higher it will lead to forward reaction and similarly a higher concentration of product leads to reverse reaction.

The parameter temperature, too has a role in determination of the reaction status. An endothermic reaction is experienced in the state of increased temperature and exothermic reaction scheme in decreased temperature state. Similarly, increased pressure causes decrease in volume of produce and vice versa.

In industrial chemical reactions, catalysts are most often used for increasing the yields of produce which has no effect on change of parameters but inert gas has an impact on reaction scheme and their implications are tabulated   below   for   quick   grasping.

Reactions	Reaction equilibrium direction
$\Delta n \rightarrow positive$	Shift to right hand side
$\Delta n \rightarrow negative$	Shift to left hand side
$\Delta n = 0$	No change in reaction scheme

1. Chemical equilibrium is a state in the course of a chemical reaction where the concentrations of both products and reactants reach the limit which prevents further deviation.

2. Le-Chatelier's principle - "If a dynamic equilibrium is disturbed by changing the conditions, the position of equilibrium moves to partially reverse the change".

3. Gibb's free energy and equilibrium - "Equilibrium is attained when the Gibbs free energy of the system is at its minimum value (assuming the reaction is carried out at constant temperature and pressure)".

4. Catalysts have an impact on the time to reach equilibrium.

Q. 3 What is meant by an Error? How errors can be detected and eliminated during a chemical analysis?

"Error" in Chemistry is defined as the difference between the true result (or accepted true result) and the measured result. If the error in the analysis is large, serious consequences may result. As reliability, reproducibility, and accuracy are the basis of analytical chemistry.

Errors fall into two basic categories:-

- **Indeterminate** (or random) **errors** are caused by uncontrollable or unknown fluctuations in variables that may affect experimental results. Indeterminate or accidental errors can arise from uncertainties in measurements.

- **Determinate errors** are those errors that are known and controllable errors e.g instrument errors, personal errors, etc. Determinate or systemic errors are known and avoidable. They can be composed of two parts that have a constant value or a proportionate value.

Types of error

- **Human Error:** Inaccuracies or mistakes by a person undertaking an experiment could be the cause of some errors. The types of human error are limitless and could include things like incorrect reading of gauges, miscalculating when diluting ingredients or similar calculations, and spillage when handling chemicals during transfer or following the wrong instructions for the experiment. Depending on what type of mistake is made and where in the process it happens will have a significant impact on the magnitude of its influence on the final solution. Human error can be minimized or eliminated by careful attention to procedures and techniques.

- **Calibration Error:** Inaccurate calibration of instruments can lead to errors in chemical experiments. Calibration is the process of adjusting or checking an instrument according to the manufacturer's instructions to ensure that the instrument gives accurate and reproducible readings. Ideally, instruments should be calibrated regularly or even every time they are used so that they do not produce errors. Some instruments or equipment will be more prone to error than others and the chemist should assess each instrument's requirement.

- **Estimated Measurement Error:** Estimating a measurement could lead to the production of an error. Some estimations are hard to eliminate. When filling a beaker with water to a specific volume there is potential to be either marginally over the mark or marginally under the mark but the chemist will estimate when they think it is spot on the mark. In an experiment that involves a color change the

moment of change will be estimated by different people at different shades of color depending on their eyesight.

- M**easurement Device Limitation Error:** The limitations of lab equipment in a lab used to measure parameters will be a potential source of error. Every instrument or device, no matter how accurate, will have limitations on accuracy associated with it. For example, a measuring flask may be provided by the manufacturer with a built-in accuracy of plus/minus 1 to 5 percent. Using this measuring flask to make measurements in a lab, therefore, introduces an error of up to 5 percent in any volume measurement.

Interpretation of experimental results requires some mathematical knowledge and the sensitivity of instruments and processes. An understanding of significant figures is often required. For example, if you are measuring the length and your instrument can read to the nearest millimeter and a calculation gives a figure to micrometers the significant figure is millimeters as there is no way of measuring smaller distances accurately.

When interpreting multiple results the values can be reported as the mean or the median. The median is the middle value and the mean is the arithmetic average. An outlier value may cause an error where an outlier is a result that is significantly different from all the other results. This could lead to a gross error being reported. The relative error can be calculated by taking the actual value minus the measured value and dividing it by the actual value and is usually expressed as a percentage.

Multiple experimental results can also be analyzed us Gaussian standardized normal curves where one standard deviation will contain 68% of results and two standard deviations will include 95% of results.

In summary, it is very unlikely that a chemical experiment will give the absolute answer. There will always be some element of error in the result. If the error is determinate it can be minimized or eliminated but indeterminate errors will not necessarily be known. The job of the chemist is to minimize or compensate for the errors to get an answer that is accurate as possible using suitable mathematical and practical strategies.

Q. 4 Describe the instrumentation and sample handling procedure.

A food analyst often has to determine the characteristics of a large quantity of food material, such as the contents of a truck arriving at a factory, a days worth of production, or the products stored in a warehouse. Ideally, the analyst would like to analyze every part of the material to obtain an accurate measure of the property of interest, but in most cases this is practically impossible. Many analytical techniques destroy the food and so there would be nothing left to sell if it were all analyzed. Another problem is that many analytical techniques are time consuming, expensive or labor intensive and so it is not economically feasible to analyze large amounts of material. It is therefore normal practice to select a fraction of the whole material for analysis, and to assume that its properties are representative of the whole material. Selection of an appropriate fraction of the whole material is one of the most important stages of food analysis procedures, and can lead to large errors when not carried out correctly.

Populations, Samples and Laboratory Samples. It is convenient to define some terms used to describe the characteristics of a material whose properties are going to be analyzed.

Population. The whole of the material whose properties we are trying to obtain an estimate of is usually referred to as the population.

Sample. Only a fraction of the population is usually selected for analysis, which is referred to as the sample. The sample may be comprised of one or more sub-samples selected from different regions within the population.

Laboratory Sample. The sample may be too large to conveniently analyze using a laboratory procedure and so only a fraction of it is actually used in the final laboratory analysis. This fraction is usually referred to as the laboratory sample.

The primary objective of sample selection is to ensure that the properties of the laboratory sample are representative of the properties of the population, otherwise erroneous results will be obtained. Selection of a limited number of samples for analysis is of great benefit because it allows a reduction in time, expense and personnel required to carry out the analytical procedure, while still providing useful information about the properties of the population. Nevertheless, one must always be aware that analysis of a limited number of samples can only give an estimate of the true value of the whole population.

Sampling Plans. To ensure that the estimated value obtained from the laboratory sample is a good representation of the true value of the population it is necessary to develop a sampling plan. A sampling plan should be a clearly written document that contains precise details that an analyst uses to decide the sample size, the locations from which the sample should be selected, the method used to collect the sample, and the method used to preserve them prior to analysis. It should also stipulate the required documentation of procedures carried out during the sampling process. The choice of a particular sampling plan depends on the purpose of the analysis, the property to be measured, the nature of the total population and of the individual samples, and the type of analytical technique used to characterize the samples. For certain products and types of populations sampling plans have already been developed and documented by various organizations which authorize official methods, e.g., the Association of Official Analytical Chemists (AOAC).

The first thing to decide when choosing a suitable sampling plan is the purpose of the analysis. Samples are analyzed for a number of different reasons in the food industry and this affects the type of sampling plan used:

Samples may be selected for official or legal requirements by government laboratories. These samples are analyzed to ensure that manufacturers are supplying safe foods that meet legal and labeling requirements. An officially sanctioned sampling plan and analytical protocol is often required for this type of analysis.

Raw materials. Raw materials are often analyzed before acceptance by a factory, or before use in a particular manufacturing process, to ensure that they are of an appropriate quality.

Process control samples. A food is often analyzed during processing to ensure that the process is operating in an efficient manner. Thus if a problem develops during processing it can be quickly detected and the process adjusted so that the properties of the sample are not adversely effected. Techniques used to monitor process control must be capable of producing precise results in a short time. Manufacturers can either use analytical techniques that measure the properties of foods on-line, or they can select and remove samples and test them in a quality assurance laboratory.

Finished products. Samples of the final product are usually selected and tested to ensure that the food is safe, meets legal and labeling requirements, and is of a high and consistent quality. Officially sanctioned methods are often used for determining nutritional labeling.

Research and Development. Samples are analyzed by food scientists involved in fundamental research or in product development. In many situations it is not necessary to use a sampling plan in R&D because only small amounts of materials with well-defined properties are analyzed.

**Q. 5 Define Carboxylic Acid and explain their nomenclature.**

The functional groups at the heart of this chapter are called **carboxylic acid derivatives**: they include carboxylic acids themselves, carboxylates (deprotonated carboxylic acids), amides, esters, thioesters, and acyl phosphates.
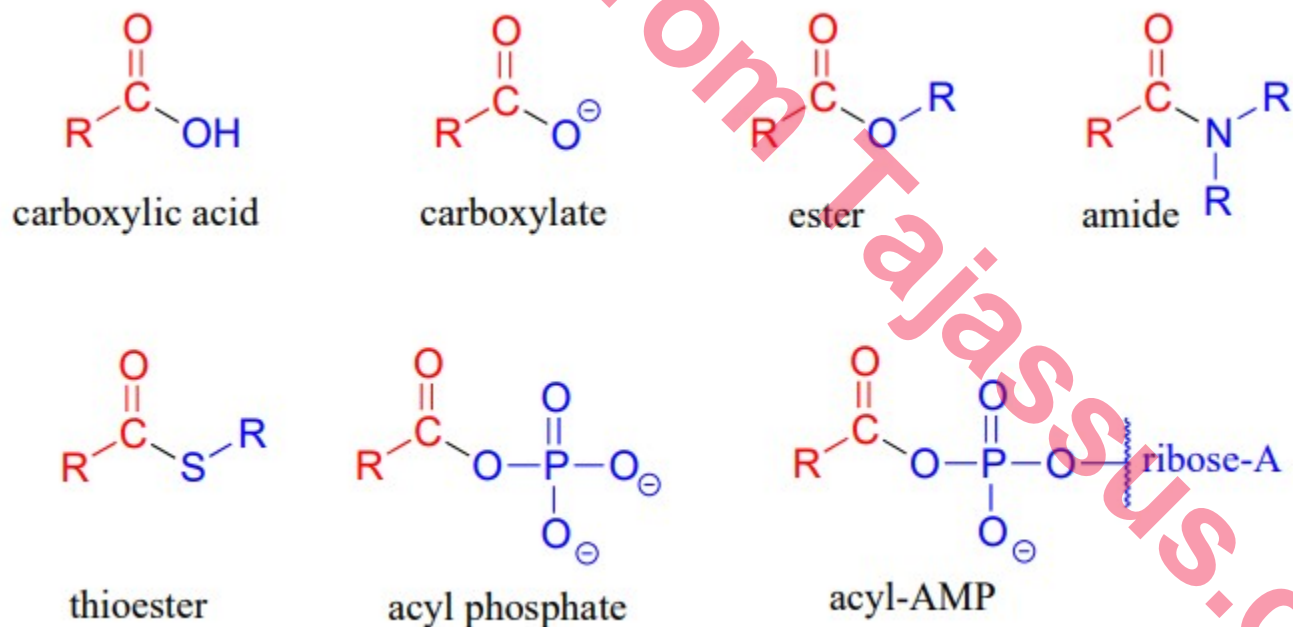
Cyclic esters and amides are referred to as **lactones** and **lactams**, respectively.
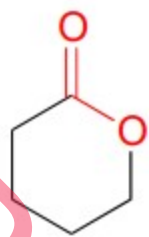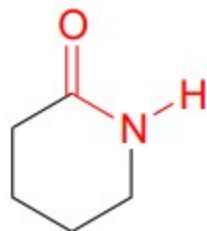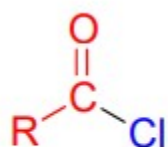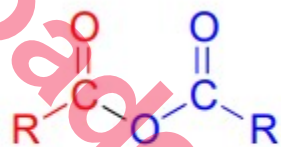
a lactone   a lactam

Carboxylic acid anyhydrides and acid chlorides, which also fall under the carboxylic acid derivative category, are not generally found in biomolecules but are useful intermediates in laboratory synthesis.


acid chloride   acid anhydride

Carboxylic acid derivatives can be distinguished from aldehydes and ketones by the presence of a group containing an electronegative heteroatom - usually oxygen, nitrogen, or sulfur – bonded directly to the carbonyl carbon. You can think of a carboxylic acid derivative as having two sides. One side is the acyl group, which is the carbonyl plus the attached alkyl (R) group. In the specific cases where R is a hydrogen or methyl, chemists use the terms formyl and acetyl group, respectively. One the other side is the heteroatom-linked group: in this text, we will sometimes refer to this component as the 'acyl X' group (this, however, is not a standard term in organic chemistry).
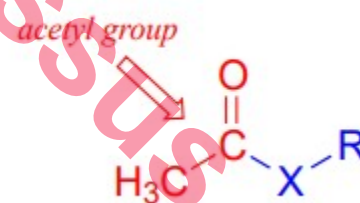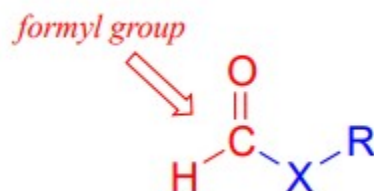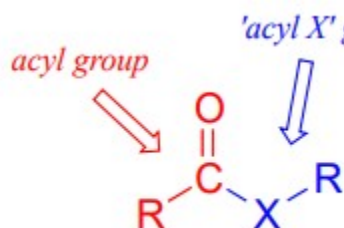

Notice that the acyl X groups are simply deprotonated forms of other functional groups linked to the acyl group: in an amide, for example, the acyl X group is an amine, while in an ester the acyl X group is an alcohol.
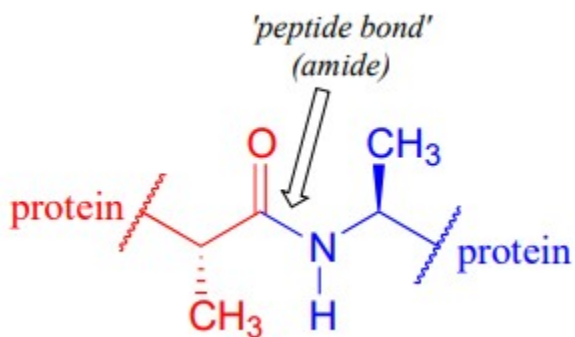
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amine = amide

acyl group **plus**

alcohol = ester
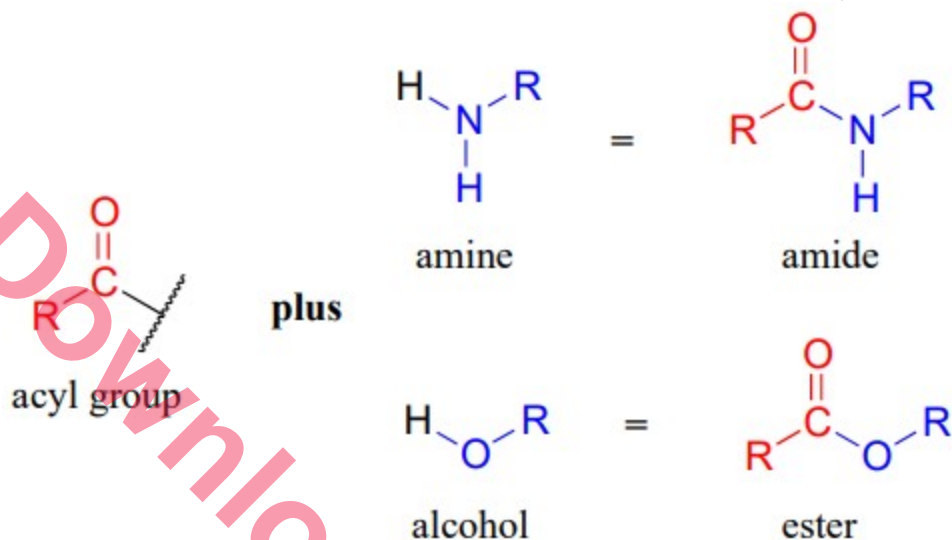
'Fatty acid' molecules such as stearate are carboxylates with long carbon chains for acyl groups.

stearate

The aromas of many fruits come from small ester-containing molecules:

pear   raspberry   apple   pineapple
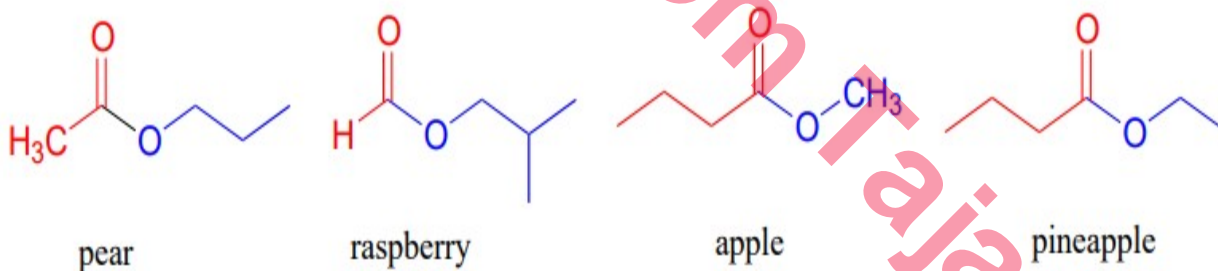
The 'peptide bonds' that link amino acids together in proteins are amides.

'peptide bond' (amide)

Acetyl-Coenzyme A, a very important two carbon (acetyl group) 'building block' molecule in metabolism, is characterized by reactions at its thioester functional group:

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thioester

acetyl-CoA