B.V.V.S

Basaveshwar Science College, Bagalkot

E-Notes

Subject: Zoology

(Study material for Undergraduate Students)

B.Sc III Sem

COURSE CODE: DSCC5ZOOT3

Molecular Biology, Bioinstrumentation & Techniques in Biology

Unit I: Process of Translation

Developed by: Smt. S. R. Sabarad

Genetic Code:

Genetic information, stored in the chromosomes and transmitted to daughter cells through DNA replication, is expressed through transcription to RNA and, in the case of messenger RNA (mRNA), subsequent translation into proteins. The pathway of protein synthesis is called **translation** because the “language” of the nucleotide sequence on the mRNA is translated into the “language” of an amino acid sequence. The process of translation requires a genetic code, through which the information contained in the nucleic acid sequence is expressed to produce a specific sequence of amino acids.

The genetic code is the set of instructions cells use to translate information from genetic material (DNA or mRNA) into amino acids. In turn, amino acids are strung together and modified to build proteins. The genetic code is sometimes called the universal code because it is used by nearly all living organisms on Earth.
There are 64 codons in the mRNA code, each consisting of three nucleotides. Most of the codons specify an amino acid. However, there is one “start” codon that encodes methionine and marks a protein’s beginning and three “stop” codons than mark the end of a protein. The nucleotides are abbreviated by the letters A, U, G, and C for adenine, uracil, guanine, and cytosine. Organisms that translate proteins directly from DNA use T for thymine rather than U for uracil. Codons are read from the 5' terminal of mRNA to the 3' end. Proteins are built from the N-terminus at **methionine to the C-terminus.**

THE GENETIC CODE

Each individual “word” in the code is composed of three nucleotide bases. These genetic words are called **codons.** There are four possible bases (U, C, A, and G) that can occupy each of the three positions in a codon, and hence there are 43-64 possible codons. Of these codons, 61 specify amino acids (of which there are only 20) and the remaining three, UAA, UAG, and UGA, are Stop codons that instruct the ribosome to cease polypeptide synthesis and release the resulting transcript.

A. Codons

Codons are presented in the mRNA language of adenine (A), guanine (G), cytosine (C), and uracil (U). Their nucleotide sequences are always written from the 5'-end to the 3'-end. The four nucleotide bases are used to produce the three-base codons. There are, therefore, 64 different combinations of bases, taken three at a time (a triplet code).

1. How to translate a codon: This table (or “dictionary”) can be used to translate any codon and,
thus, to determine which amino acids are coded for by an mRNA sequence. For example, the codon 5'-AUG-3' codes for methionine. [Note: AUG is the initiation (start) codon for translation.] Sixty one of the 64 codons code for the 20 common amino acids.

2. Termination (“stop” or “nonsense”) codons: Three of the codons, UAG, UGA, and UAA, do not code for amino acids, but rather are termination codons. When one of these codons appears in an mRNA sequence, synthesis of the polypeptide coded for by that mRNA stops.

Characteristics of the genetic code include the following:

1. Specificity: The genetic code is specific (unambiguous) that is, a particular codon always codes for the same amino acid.

2. Universality: The genetic code is virtually universal, that is, its specificity has been conserved from very early stages of evolution, with only slight differences in the manner in which the code is translated. (An exception occurs in mitochondria)

3. Degeneracy: The genetic code is degenerate (sometimes called redundant). Although each codon corresponds to a single amino acid, a given amino acid may have more than one triplet coding for it. For example, arginine is specified by six different codons. Only Met and Trp have just one coding triplet.

4. Non-overlapping and comma less: The genetic code is non-overlapping and comma less, that is, the code is read from a fixed starting point as a continuous sequence of bases, taken three at a time. For example, AGCUGGAUACAU is read as AGC/UGG/AUA/CAU without any "punctuation" between the codons. Consequences of altering the nucleotide sequence: Changing a single nucleotide base on the mRNA chain (a "point mutation") can lead to any one of three results.

5. Silent mutation: The codon containing the changed base may code for the same amino acid. For example, if the serine codon UCA is given a different third base—U—to become UCU, it still codes for serine. This is termed a "silent" mutation.

6. Missense mutation: The codon containing the changed base may code for a different amino acid. For example, if the serine codon UCA is given a different first base—C—to become CCA, it will code for a different amino acid, in this case, proline. The substitution of an incorrect amino acid is called a "missense" mutation.

7. Nonsense mutation: The codon containing the changed base may become a termination codon. For example, if the serine codon UCA is given a different second base—A—to become UAA, the new codon causes termination of translation at that point, and the production of a shortened (truncated) protein. The creation of a termination codon at an inappropriate place is called a "nonsense" mutation.

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Economic Zoology

Vermicomposting Unit - IV

Smt. S. R. Sabarad, HOD, Department of Zoology, Basaveshwar Science College, Bagalkot

Earthworms:

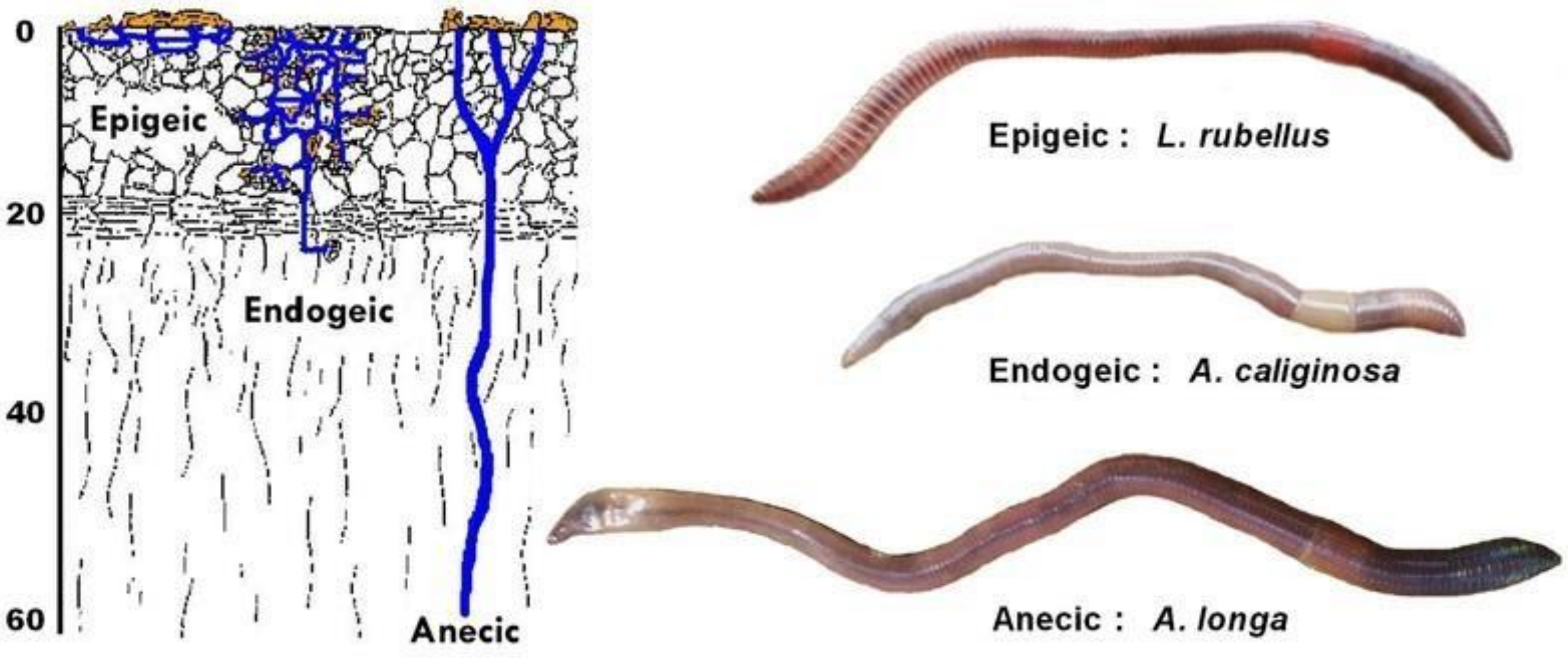
- There are about 3000 species of earthworms in the world which are adapted to a range of environment, in tropical to temperate region.
- About 418 species of earthworms present in India.
- India harbors about 11.1% of the global earthworm diversity.
- The Indian earthworm fauna is predominantly composed of native species, which constitute about 89% of total earthworm diversity in the country.
- Around 45 exotic peregrine worms have been introduced into India.

Types of Earthworms

- Three ecological categories of earthworms - epigeics, endogeics and anecics.

•The anecics and endogeics are known as ‘soil ecosystem engineers’ and their impact on soils is great and may influence properties and processes at the ecosystem level.

•The functional role of epigeics is primarily that of ‘litter transformers’, like other litter invertebrates.



Epigeics

- Epigeic species grind and partially digest surface litter, rarely ingesting soil particles.

- The soils are affected indirectly via changes in the litter, the effects of epigeic earthworms are not truly ***drilospheric***.
- Their mode of litter processing in natural systems results in greater nutrient leaching into the soil.
- The epigeics feed purely on litter and generally have a short *gut transit time* they probably depend on a rapid response of gut microbes to aid in digestion.

Endogeics

- Endogeics are the most prevalent earthworms (in biomass) in most tropical environments, often being the only group present, particularly in agro ecosystems.
- Endogeics are oeophagous earthworms that feed on subsurface soil horizons and on soil organic matter of different qualities.
- They produce surface and below-ground casts.
- Endogeic casts with generally more clay and more organic matter than undigested soil, contain and release significant amounts of nutrients.

- Fresh casts of *Pontoscolex corethrurus* may have 2-8 times more inorganic P and NH4 than undigested soil.
- This N may result from selective ingestion of richer soil portions, microbial mineralization, enteronephridial N excretions or a symbiotic N2 (Dinitrogen) fixation in the gut.
- Fungal hyphae, active protozoa, algae, myxomycetes and nematodes may be digested, while encysted or protected forms survive gut passage and then rapidly proliferate in casts.

Anecics

- Anecics the dominant earthworms (in biomass) in many temperate region soils are primarily vertically burrowing species.
- They feed on surface litter and more or less are permanent refuges in underlying soil horizons.

- They often produce characteristic surface features called "**middens**" which are circular "mound-shaped" region around a surface of the burrow's opening which is a mixture of surface organic materials and soil.
- These are thought to act as "external rumens," where microbes and fauna attracted to this 'hot-spot' enhance decomposition of undigested litter and organic fragments in casts, probably due to fungal colonization of these substrates.
- The feeding and casting habits of anecics may deeply influence soil characteristics up to 1m depth.
- The translocation of litter, mucus excretions, air penetration and selection of soil particles enrich the burrow walls with organic matter and plant available nutrients (N, P, K and Ca).

Ecological role and Economic importance of Earthworms:

- The microorganisms and earthworms act symbiotically to accelerate and enhance the decomposition of organic matter.
- Earthworms in general are greatly resistant to many pesticides and concentrate the pesticides and heavy metals in their tissues.
- They also inhibit the soil borne pathogens and work as a detoxifying agent for polluted soil.
- Earthworms can be used for effluent treatment and heavy metal and pesticides removal from industrial and agricultural wastes.
- Earthworm promotes the growth of ‘beneficial decomposer bacteria’ in waste biomass.
- Earthworms are the most important soil invertebrate in the soil ecosystem in terms of biomass and activity, often considered as ecosystem engineer.
- Earthworms are not essential to have in the soil, but their presence can be an indicator of good soil quality.

- Earthworms improve the physical structure of soil, improve water filtration rates and absorption rates, helping the soil to drain better.
- The tunnelling activity of earthworms also improves soil aeration, porosity and permeability.
- The feeding and casting habits of anecics may deeply influence soil characteristics up to >1m depth.
- The translocation of litter, mucus excretions, air penetration and selection of soil particles enrich the burrow walls with organic matter and plant available nutrients (N, P, K and Ca).

Vermiculture – definition, scope and importance:

Vermiculture:

- Vermiculture means scientific method of breeding and raising earthworms in controlled conditions.

Vermitechnology:

- Vermitechnology is the combination of verminculture and vermicomposting.
- Earthworm can be used for development of arable soils, break down of plant organic matter, aeration and drainage.
- Also for production of useful products like vermifertilizer and worm tissue for animal feed.

Vermicomposting – applications, future perspectives:

- ‘Gold from garbage’ and ‘Queen of compost’
- Vermicomposting is a method of making compost, with the use of earthworms, which generally live in soil, eat biomass and excrete it in digested form. This compost is generally called Vermicompost or Wormicompost.
- **Epigeics** (surface feeders) are important in vermicomposting. The epigeics such as *Eisenia foetida* and *Eudrilus eugeniae* are exotic worms and *Perionyx excavatus* is a native one being used for vermicomposting in India.

- **Epianecic** are feeders on leaf litter and soil at upper layers of soil. This group such as *Lampito mauritii* is indigenous and is active in in-situ decomposition of organic wastes and residues in soil.

- Both **epigeics** and **epianecics** groups of earthworms are slender, shorter in length and red to dark brown in colour. They have high reproduction activity and efficient in recycling of organic materials.
- Increased attention has been paid to *Eisenia foetida* and *Eudrilus eugeniae* which have been found to be potential agent in vermicomposting of wide range of agricultural wastes and can grow at a wide range of temperature varying from 0-40 ◦C. However, the optimum temperature ranges from 20-30 ◦C.

- Materials consumed by worms undergo physical breakdown in the gizzard resulting in particles <2 µ, giving thereby an enhanced surface area for microbial processing.
- This finally ground material is exposed to various enzymes such as protease, lipase, amylase, cellulase and chitinase secreted into lumen by the gut wall and associated microbes.
- These enzymes breakdown complex biomolecules into simple compounds.

- Only 5-10% of the ingested material is absorbed into the tissues of worms for their growth and rest is excreted as cast.
- Mucus secretions of gut wall add to the structural stability of vermicompost.

Vermicompost preparation

- Basic raw materials: Any organic material generated in the farm like wheat / rice straw, leaf fall, Paddy husk, etc.
- Starter: Cow dung , Biogas slurry, or urine of cattle.
- Earthworm sp.: Earth worms (Species: *Eisenia foetida*)
- Thatched roof/vermi shed.

Procedure:

- It is mostly prepared in either pit or heap method.
- The dimensions either heap or pit are 10 x 4 x 2 feet.
- The length and width can be increased or decreased depending on the availability of material but not the depth because the earthworms’ activity is confined to 2 feet depth only.
- First of all select a site which is not under any economic use and is shady and there is no water stagnation. The site should be near to a water source.
- 1st layer: bedding material of 1" thick with soft leaves
- 2nd layer: 9" thick organic residue layer finely chaffed material
- 3rd layer: Dung + water equal mixture of 2" layer.
- Continue the layer up to pile to ground level in the case of pit method and up to 2′ in heap or surface bed method.

- Protect the worms against natural enemies like ants, lizards, snakes, frogs, toads etc., Maintain proper moisture and temperature by turnings and subsequent staking.
- At the day of 24th, 4000 worms are introduced in to the pit [1m^2 =2000 worms] without disturbing the pit by regular watering the entire raw material will be turned into the vermicompost in the form of worm excreta.
- The turnover of the compost is 75% [the total material accommodated in the pit is 1000 kg; the out turn will be 750 kg]
- In-situ vermicomposting can be done by direct field application of vermicompost at 5 t/ha followed by application of cow dung (2.5 cm thick layer) and then a layer of available farm waste about 15 cm thick.
  Irrigation should be done at an interval of 15 days.

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- *ZL(OE)-02: Economic Zoology Vermicomposting Unit - IV*
- *https://www.aisectuniversityjharkhand.ac.in/PDFDoc/StudyNotes/B.SC%20Zoology/B.Sc%20Zoology%20(Sem%20V)/Sem%20V%20DSE-1%20Economic%20Zoology.pdf*

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B.Sc I Sem

COURSE CODE: 21BSC1C1ZOO1L

Molecular Biology, Bioinstrumentation & Techniques in Biology

Unit IV: Molecular Techniques

Developed by: Smt. S. R. Deshpande

SDS-PAGE (Sodium Dodecyl Sulfate Polyacrylamide Gel Electrophoresis):
SDS-PAGE is a powerful and widely used technique in molecular biology and biochemistry for separating and analyzing proteins, providing valuable information about their size and purity.
SDS-PAGE is a powerful and versatile technique for protein separation and analysis. It is widely used in various research fields and is a valuable tool for understanding the structure and function of proteins.

1. Sample Preparation:

- Proteins are extracted from the desired sample using appropriate lysis buffers and homogenization techniques.
- The extracted protein concentration is determined using assays like Bradford or BCA.
- Protein samples are then denatured by heating with sodium dodecyl sulfate (SDS) and a reducing agent like β-mercaptoethanol. This disrupts protein folding and disulfide bonds, resulting in linear polypeptide chains with a negative charge proportional to their length.

2. Gel Preparation:

- Two types of gels are used:
  - **Resolving gel:** This gel separates proteins based on their size. It is made of a cross-linked polyacrylamide matrix with pore sizes determined by the acrylamide concentration.
  - **Stacking gel**: This gel helps to concentrate the protein samples before entering the resolving gel. It has a lower acrylamide concentration and a larger pore size than the resolving gel.
- The gels are prepared by mixing acrylamide, bisacrylamide, buffer, and initiators (TEMED and APS). The resolving gel is poured first, followed by the stacking gel after the resolving gel has partially polymerized.
- Inserting Comb: After pouring the gel, a comb is inserted to create wells for loading the protein samples.
- **Polymerization:** The gel is allowed to polymerize, forming a porous matrix.

3. Gel Loading and Electrophoresis:

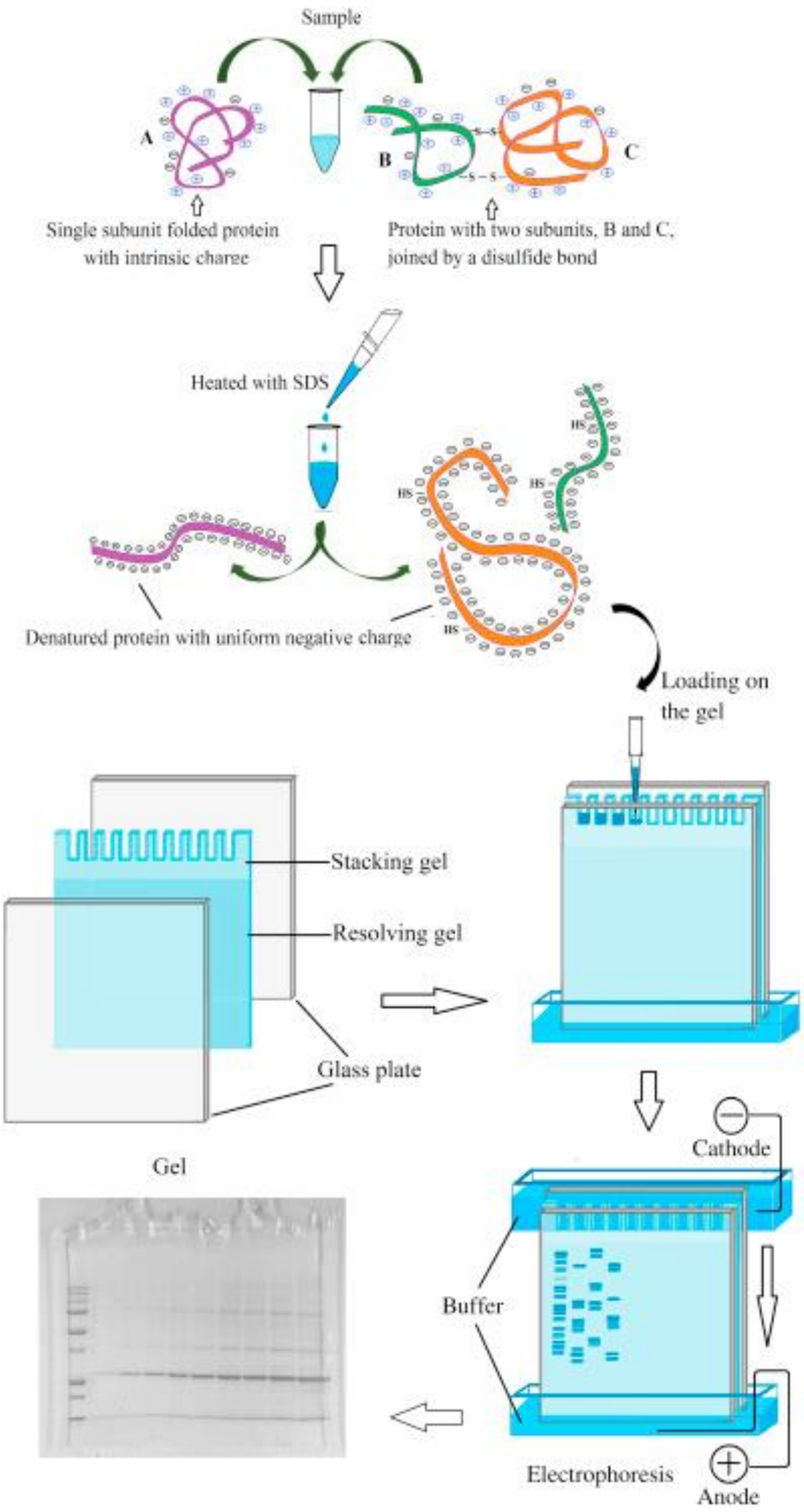
- The protein samples are mixed with a loading buffer containing SDS and a tracking dye (e.g., bromophenol blue).
- The samples are carefully loaded into the wells of the stacking gel.
- The electrophoresis apparatus is assembled with the gel and a running buffer containing SDS and Tris-glycine.
- An electric current is applied across the gel, causing the negatively charged proteins to migrate towards the positive electrode.
- Smaller proteins move through the gel pores more easily and migrate faster than larger proteins.

4. Staining and Visualization:

- After electrophoresis, the proteins are stained with a dye that binds to protein molecules. **Coomassie Brilliant Blue** is commonly used for this purpose.
- The gel is then destained to remove excess stain and reveal protein bands.
- The protein bands can be visualized under ultraviolet light and photographed for analysis.

5. Data Analysis:

- The size of the protein bands can be estimated by comparing them to a protein ladder of known molecular weights.
- The relative abundance of different proteins in the sample can be determined by measuring the intensity of the protein bands.
- The results of SDS-PAGE can be used to identify unknown proteins, analyze protein expression levels, and study protein modifications.



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(Study material for Undergraduate Students)

B.Sc I Sem

COURSE CODE: 21BSC1C1ZOO1L

Cytology, Genetics and Infectious Diseases

Unit I: Endomembrane System

Developed by: Smt. S. R. Deshpande

Endomembrane System:

The endomembrane system separates the cell into different compartments, or organelles, such as the nucleus, the endoplasmic reticulum (ER), the Golgi apparatus, and lysosomes. The endomembrane system is derived from the ER and flows to the Golgi apparatus, from which lysosomes bud.

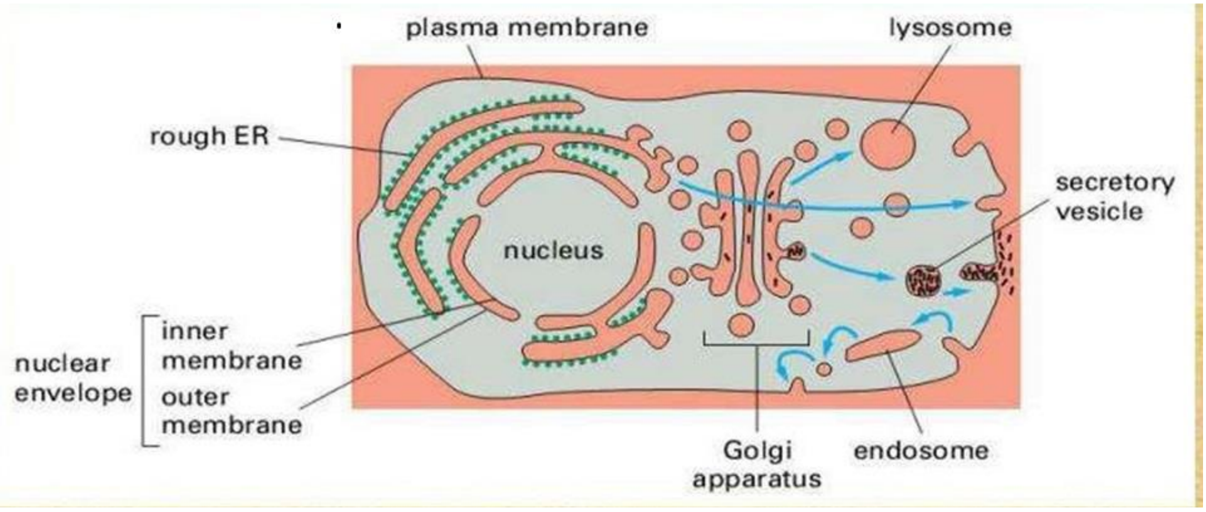
The endomembrane system includes the **Endoplasmic Reticulum (ER), Golgi Apparatus, And Lysosomes.** Vesicles also allow the exchange of membrane components with a cell's plasma membrane.

Protein Sorting:

Protein targeting or **protein sorting** is the biological mechanism by which proteins are transported to their appropriate destinations in the cell or outside it.

Proteins can be targeted to the inner space of an organelle, different intracellular membranes, plasma membrane, or to exterior of the cell via **secretion.**

This delivery process is carried out based on information contained in the protein itself.



In 1970, ***Gunter Blobel*** conducted experiments on the translocation of proteins across membranes. He was awarded that many proteins, have signal sequence, that is short amino acid sequence at one end that functions like postal code for the target organelle.

Endoplasmic Reticulum- The vesicular network starts from nuclear membrane and spread throughout the cytosol constitutes endoplasmic reticulum.

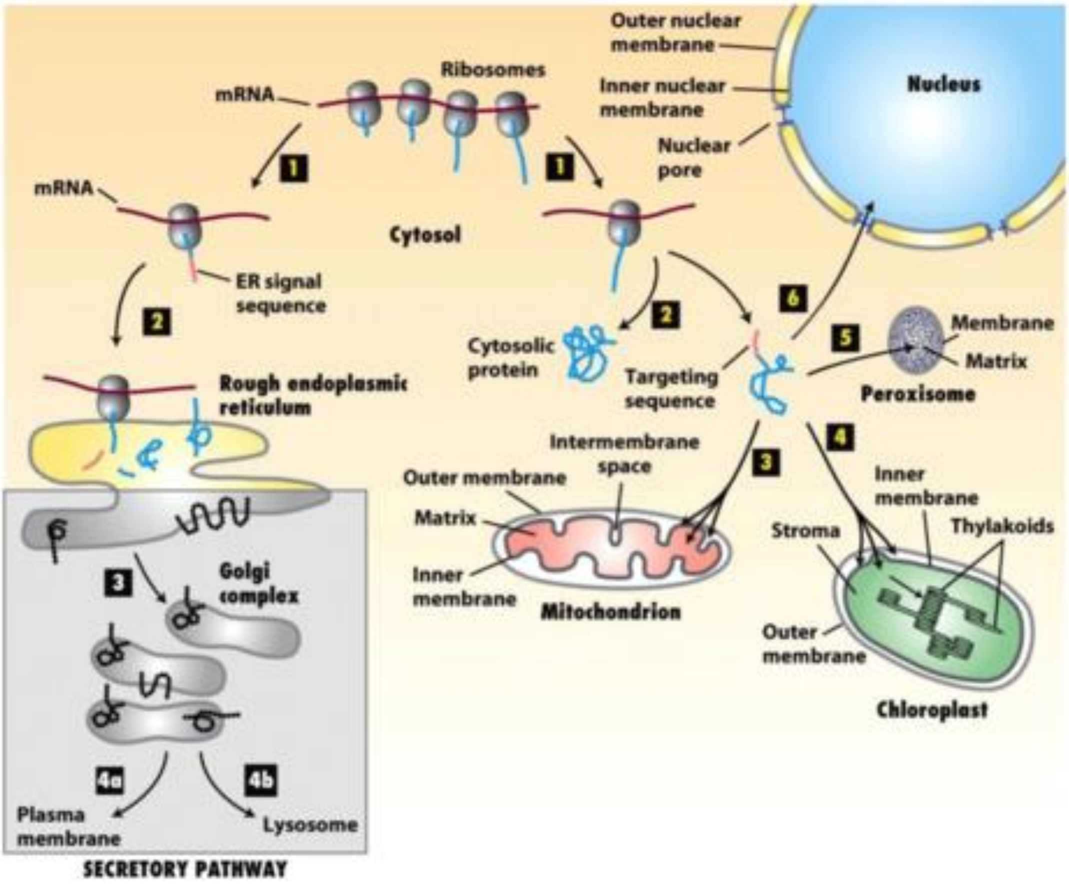
Protein synthesis on ribosome attached to **RER** are sorted into 3 different categories, such as **integral membrane proteins**, **proteins for secretion** and **protein destined** for different organelles. Proteins are synthesized with a n-signal peptide and these signal peptides are recognized by signal recognition particle on the target organelles. The proteins without any signal peptide tags are supposed to remain in the cytosol. The translocation starts while the protein is still being synthesized on the ribosome. Proteins targeted for ER, Golgi apparatus, plasma membrane, lysosome, vacuole and extracellular space uses the SRP-dependent pathway and are translocated **Co-Translationally.**

- The **N-terminal signal sequence** of these proteins is recognized by a signal recognition particle (SRP), while the proteins being translated in the free ribosome.

- The ribosome-protein complex is transferred to a SRP receptor on the ER and the synthesis pauses.
- There, the nascent protein is inserted into the translocon that passes through the ER membrane. Transfer of the ribosome-mRNA complex from the SRP to the translocon opens the gate on the translocon and allows the translation to resume.
- The signal sequence is immediately cleaved from the polypeptide once it has been translocated into the ER by signal peptidase in secretory proteins. Within the ER, **chaperone (mammalian protein)** helps protein to fold correctly.
- From **ER, proteins** are transported in vesicles to the **Golgi apparatus** where they are further processed and sorted for transport to endosomes, lysosomes, plasma membrane or secretion from the cell.
- The proteins for ER will have various ER retention signals to keep them in the ER itself. Proteins are sorted to their locations with the help of an address signal present in the primary structure level. Each organelle has a mechanism to identify its own proteins. In this section, important protein localization sites like nucleus, mitochondrion, chloroplast, peroxisome, and secretory proteins.
- The Endoplasmic Reticulum is the first branching point in protein sorting.
- Most of the proteins targeted for secretion, Golgi apparatus, plasma membrane, vacuole, lysosome are translated on the ribosomes bounded to the Endoplasmic Reticulum and they enter into the ER **co-translationally (CTT)**. Only a few proteins enter the ER **post-translationally (PTT).**
- The protein translation starts at the free ribosomes in the cytosol. The synthesis continues till the sorting signal which is present in the **N-terminal** emerges.
- This sorting signal is recognized by signal recognition particle. The **SRP (Single Recognition Particle)** binds to the sorting signal and the translation pauses.
- The complex of **SRP**, ribosome, polypeptide chain and mRNA move to the ER and the polypeptide chain enters the ER through **translocon.**
- The **translocon** is a protein complex containing various components used for protein translocation.
- The SRP receptor of the **translocon** binds with the SRP, the ribosome receptor binds with the **ribosome** and hold it in the correct position, the pore protein forms the channel through which the growing polypeptide enter the ER lumen, the signal peptidase cut the signal once it enters the ER.
- After the **SRP** and ribosomes are bound by SRP receptor and ribosome receptor respectively, GTP binds to the complex of SRP and SRP receptor and the translation resumes.
- This causes the transfer of the signal sequence into the channel of pore protein.
- Then the GTP is hydrolysed and the SRP is released. While the sorting signal remains bound at the **pore protein,** the polypeptide grows into a loop and translocate into the ER lumen
- When the polypeptide synthesis is finished, the signal peptidase cleaves off the sorting signal, releasing the polypeptide into the ER lumen.
- After this, the ribosome detaches from the ER and dissociate into its subunits, and the mRNA is released.

- Inside the ER, the polypeptide chains are folded into their native forms usually with the help of molecular chaperones, which controls the quality of protein folding.
- Integral membrane proteins of the plasma membrane or the membranes of the ER, Golgi apparatus, and lysosome are first inserted into the membrane of ER.
- These proteins do not enter the lumen **Co-Translationally** but anchored to the ER membrane by membrane spanning α helices that stop transfer of the growing polypeptide chain across the membrane.
- Proteins travel along the secretory pathway in transport vesicle, which bud from the membrane of one organelle and then fuse with the membrane of another.
- The proteins are exported from the ER in vesicles that bud from the **transitional ER** and carry their cargo through the ER-Golgi intermediate compartment and then to Golgi apparatus.
- The proteins targeted for the ER has a retention signal in their **C- terminal** that makes them come back to the ER even if they are exported from the ER.
- **A signal sequence** on a growing protein will bind with a **Signal Recognition Particle (SRP).**
- This slows protein synthesis. The **SRP** then binds to a location on the surface of the nearby ER.
- Then, the **SRP** is released, and the protein-ribosome complex is at the correct location for movement of the protein through a translocation channel.
- A multi-step schematic shows the process of translation as it occurs in the **endoplasmic reticulum (ER).**
- A signal recognition particle **(SRP)** is represented as an orange triangle and is shown binding to the newly synthesized polypeptide's blue terminal signal sequence.
- The ER membrane, which is a lipid bilayer, is shown directly below the large ribosomal subunit. The triangular **SRP** docks to a triangle-shaped cavity in an orange SRP receptor protein.
- The SRP receptor protein is positioned in the ER membrane beside a closed protein channel, called the translocon.
- A GTP molecule is bound to the SRP, and a second GTP molecule is bound to the SRP receptor; the GTP molecule bound to SRP. Next, the growing polypeptide, which is still attached to the ribosome, is transferred to the translocon, which opens. The growing polypeptide is threaded through the pore.
- The GTP molecules on the SRP and SRP receptor have each been hydrolysed to form GDP and a free phosphate molecule, and both the SRP and the SRP receptor have dissociated from the translocon.
- The growing polypeptide travels the length of the membrane channel and dangling into the ER from the ribosome attached to the mRNA molecule above.
- After the entire polypeptide has passed through the translocon, the growing polypeptide is completely detached from the ribosome, which has disassembled, and the polypeptide now appears as a curled-up structure floating loose inside the ER.

- Transport of molecules within a cell and out of the cell requires a complex endomembrane system.
- Endocytosis occurs when the cell membrane engulfs particles (dark blue) outside the cell, draws the contents in, and forms an intracellular vesicle called an endosome.
- This vesicle travels through the cell, and its contents are digested as it merges with vesicles containing enzymes from the Golgi. The vesicle is then known as a lysosome when its contents have been digested by the cell.
- **Exocystosis** is the process of membrane transport that releases cellular contents outside of the cell.
- Here, a transport vesicle from the Golgi or elsewhere in the cell merges its membrane with the plasma membrane and releases its contents. In this way, membranes are continually recycled and reused for different purposes throughout the cell.
- Membrane transport also occurs between the endoplasmic reticulum and the Golgi.



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E-Notes

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B.Sc I Sem

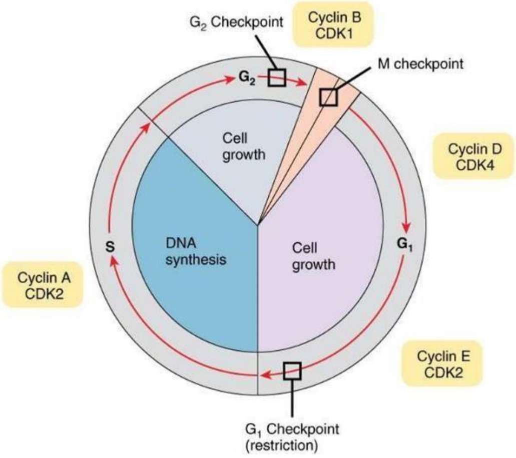
COURSE CODE: 21BSC1C1ZOO1L

Cytology, Genetics and Infectious Diseases

Unit II: Cell cycle, Cell Division and Cell Signaling

Developed by: Smt. S. R. Deshpande

Introduction to Cell cycle and its regulation, apoptosis



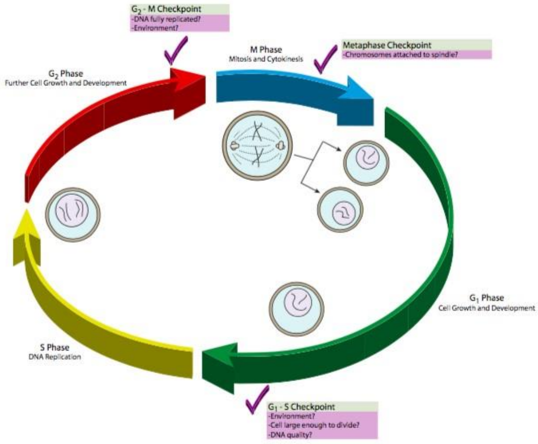
1.Interphase- The time between the **end of telophase and the beginning of the next M phase is called the interphase**. It is a long stage that lasts for 10 to 30 hours. During this phase the cell grows by synthesizing biological molecules such as lipids, proteins, carbohydrates, nucleic acids.
Interphase is further divided into **three sub phases** or periods:
first gap or **G1 phase**, synthetic or **S phase** and second gap or **G2 phase.**

(i) **G_1 phase-** The **gap between previous mitosis and beginning of DNA synthesis** is represented by G_1 phase. In this stage initial growth of a newly formed cell takes place. Various biological molecules (carbohydrates, proteins, lipids, including some non-histones, RNAs) are synthesized in this phase. Normal metabolism is carried out for the preparation for DNA replication that is to take place next to it. DNA synthesis does not occur in this phase.

(ii) **S Phase-** During this **phase duplication of each chromosome** take place by replication of new DNA molecule on the template of the existing DNA. Synthesis of histone proteins and their mRNA, some nonhistone proteins and formation of new nucleosome also occur in Sphase only. In most of the eukaryotes the S-phase lasts for 6 to 8 hours.

(iii) **G_2 Phase-** G_2 phase is the gap between DNA synthesis and nuclear division. RNA transcription and protein synthesis continues during this phase. Further growth of the cell and preparation for its division also takes place in this stage. During this stage the cytoplasmic organelles such as centrioles, mitochondria and Golgi apparatus are doubled, proteins for spindle and asters are synthesized and active metabolism stores energy for the next mitosis. The G_2 phase in most cells lasts for 2 to 5 hours.

Regulation of the Cell Cycle:
Daughter cells must be exact duplicates of the parent cell. Mistakes in the duplication or distribution of the chromosomes can lead to mutations that may be passed forward to every new cell produced from the abnormal cell. To prevent a compromised cell from continuing to divide, there are internal control mechanisms that operate at three main **cell cycle checkpoints.**



Cell Cycle Checkpoints. The cell cycle is controlled at three checkpoints. The integrity of the DNA is assessed at the **G1-S checkpoint**. Proper chromosome duplication is assessed at the **G2-M checkpoint**. Attachment of each kinetochore to a spindle fibre is assessed at the **M checkpoint**.

The G1-S Checkpoint

The G1-S checkpoint determines whether all conditions are favourable for cell division to proceed and for DNA replication to occur during S phase. There is a check for damage to the **genomic DNA** and ensure there is space for a near cell at the G1S checkpoint. A cell that does not meet all the requirements will “arrest” in G1 and try repair DNA damage. If, during cell cycle arrest, the cell can meet the G1-S checkpoint criteria, the cell cycle will proceed to the **S phase**. If not, the cell will undergo **apoptosis (programmed cell death).**

The G2-M Checkpoint

The G2-M checkpoint bars the entry to the mitotic phase if certain conditions are not met. As in the G1-S checkpoint, cell size and protein reserves are assessed. The most important role of the G2 checkpoint is to ensure that all the chromosomes have been replicated and that the replicated DNA is not damaged. Also, like the G1-S checkpoint, the cell cycle will arrest at the G2-M transition

The M Checkpoint

The M checkpoint occurs near the end of the **metaphase stage of mitosis**. The M checkpoint is also known as the **spindle checkpoint** because it determines if all the sister chromatids are correctly attached to the spindle microtubules. Because the separation of the sister chromatids during anaphase is an irreversible step, the cycle will not proceed until the **kinetochores** of each pair of sister chromatids are firmly anchored to spindle fibres arising from opposite poles of the cell. As with the previous checkpoints, cells that cannot proceed past this checkpoint will be eliminated by **apoptosis.**

Positive Regulation of the Cell Cycle:

Two groups of proteins, called **cyclins** and **cyclin-dependent kinases (CDKs)**, are termed, positive regulators. They are responsible for the progress of the cell through the various checkpoints. The levels of **cyclin proteins** fluctuate throughout the cell cycle in a predictable pattern. Both external and internal signals trigger increases in the trigger the expression of **cyclins** that are specific to each stage of the **cell cycle.** After the cell moves to the next stage of the cell cycle, the cyclins that were active in the previous stage are polyubiquitinated and degraded by the **proteasome.**

Apoptosis

Apoptosis, also called programmed cell death, in biology, a mechanism that allows cells to self-destruct when stimulated by the appropriate trigger. Apoptosis can be triggered by mild cellular injury and by various factors internal or external to the cell; the damaged cells are then disposed of in an orderly fashion. As a morphologically distinct form of **programmed cell death**, apoptosis is different from the other major process of cell death known as necrosis. Apoptosis involves condensation of the nucleus and cytoplasm, followed by cellular partitioning into well-defined fragments for disposal. In multicellular organisms, cell number normally results from the rate of cell production minus the rate of apoptosis.

References: *https://www.onlinebiologynotes.com/checkpoints-and-regulation-of-cellcycle%ef%bb%bf/*

https://www.bdbiosciences.com/content/dam/bdb/marketingdocuments/BD_Reagents_Apoptosis_Brochure.pdf

Reference: https://www.techtarget.com/searchcontentmanagement/definition/web-content-management-WCM

What is a web content management system (WCMS)?

A web content management system (WCMS) is a type of content management system (CMS) that provides an organization with a way to manage digital information on a website through creating and maintaining content without prior knowledge of web programming or mark up languages.

Managing web content effectively can have useful applications in the enterprise, producing insights for decision-making and delivering results, as well as value.

How does a WCMS work?

A WCMS helps users maintain, control, change and reassemble content on a webpage. Users store content within a database and can assemble the content using a flexible language such as Extensible Markup Language (XML) or .Net. Users can access the WCMS through a web browser, then edit the content and maintain control of the layout from that browser-based interface.

A WCMS has the following two parts:

- **Content management application (CMA).** This user interface lets users -- such as marketers and content creators -- design, create, modify and remove content from the website without requiring help from the IT department.
- **Content delivery application (CDA).** This provides back-end services that take the content that users create in the CMA and turn it into a website that visitors can access.

An organization can run a WCMS in its own data center or in the cloud.

Why use a WCMS?

A WCMS helps businesses create, manage and publish content on websites, which are essential marketing channels. Typically, digital marketing tactics such as email, social media, print and other advertisements direct the customer to the company website, so it's important for the business to have and maintain a web presence. A WCMS is the technology that powers websites that focus on content creation and sharing -- such as blogs and portfolios. However, organizations can also use a WCMS for other purposes, including online stores or online forums.

Capabilities and features

A WCMS typically enables users to do the following:

- Design, create and maintain personalized content for a website.
- Review and approve content prior to publication.
- Use an automated publishing process.

A WCMS generally includes the following features:

- **Automated, standard templates.** Users can easily add new or existing content, rather than having to design their own templates.
- **Access control.** Administrators can control who has access to a page on a website.
- **Scalable expansion.** Organizations can expand an implementation across multiple domains.
- **Web-based editing tools.** Users can create and customize content, such as adding titles and headers to improve content structure or designing web pages with drag-and-drop tools.
- **Personalization tools.** Users can create a customized digital experience. Marketers and content developers can present targeted content pages to users based on their customer profiles and past behaviors.
- **Plug-in.** Plugins or modules extend a site's functionality.
- **Software updates.** These keep the WCMS up to current web standards.
- **Workflow management.** This lets authorized users review and approve content before publishing.
- **Collaboration tools.** Multiple users can modify content and include features for gathering user feedback.
- **Document management.** Businesses can manage the document lifecycle, including creation, revisions, publication, archive and removal.
- **Multilingual.** Organizations can display content in various languages.
- **Versioning.** Editors can retrieve previous versions of content.

Advantages of using a WCMS

A WCMS offers organizations the following benefits:

- **Low cost.** A WCMS is typically inexpensive, often being free or offering subscriptions that outweigh overall costs.
- **Ease of use.** Most WCMS options are user-friendly and let people who don't have a technical coding background create or maintain content.
- **Ease of customization.** A WCMS creates a universal layout that lets beginner users create and customize front ends easily.
- **Workflow management.** Administrators can control and personalize workflow management in a WCMS. Some WCMS options let administrators set up their own workflow management rules and provide them with a series of steps to set up each task.
- **Search engine optimization (SEO).** A WCMS gives businesses the editing tools required to improve search engine ranking. Users can easily create content with the correct keywords, provide meta information -- such as description, keywords and alternative text for images -- and link content within the text.

Disadvantages of using a WCMS

On the other hand, a WCMS isn't the best fit for all organizations. The disadvantages of a WCMS include the following:

- **High cost for larger implementations.** A WCMS can be expensive for larger companies because it can require extensive training and certifications. WCMS maintenance can also be expensive because the software often requires upgrades and licensing updates.
- **Latency issues.** Larger systems can become slower over time if the business doesn't keep the hardware up to date or if the cache files grow too large.
- **Security risks.** If an administrator doesn't regularly patch the WCMS for security threats, it remains vulnerable to hackers. To minimize security risks, administrators must monitor and maintain the many moving parts of a WCMS -- such as the web server software, MySQL and any plugins or add-ons.

Department of Computer Science

Staff Name: Smt. Naina J. Kalyanshetti

Class: B.C.A IV semester

Subject Name: Python Programming

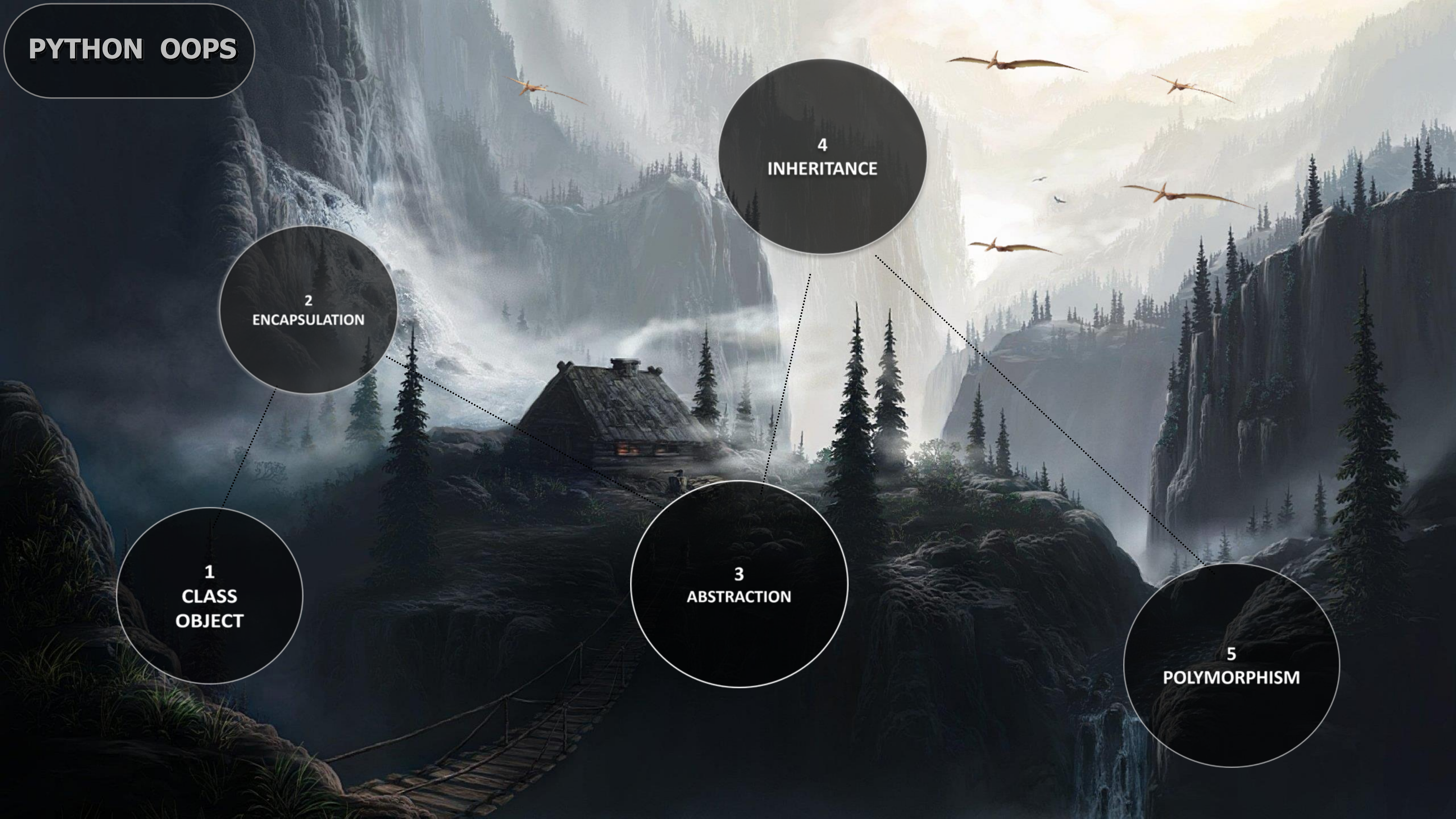
Course Code: 21BCA3C10L

OBJECT
ORIENTED
PROGRAMMING
STRUCTURE

OOPS

1. CLASS
2. OBJECT
3. ENCAPSULATION
4 ABSTRACTION
5. INHERITANCE
6. POLYMORPHSM

PYTHON OOPS



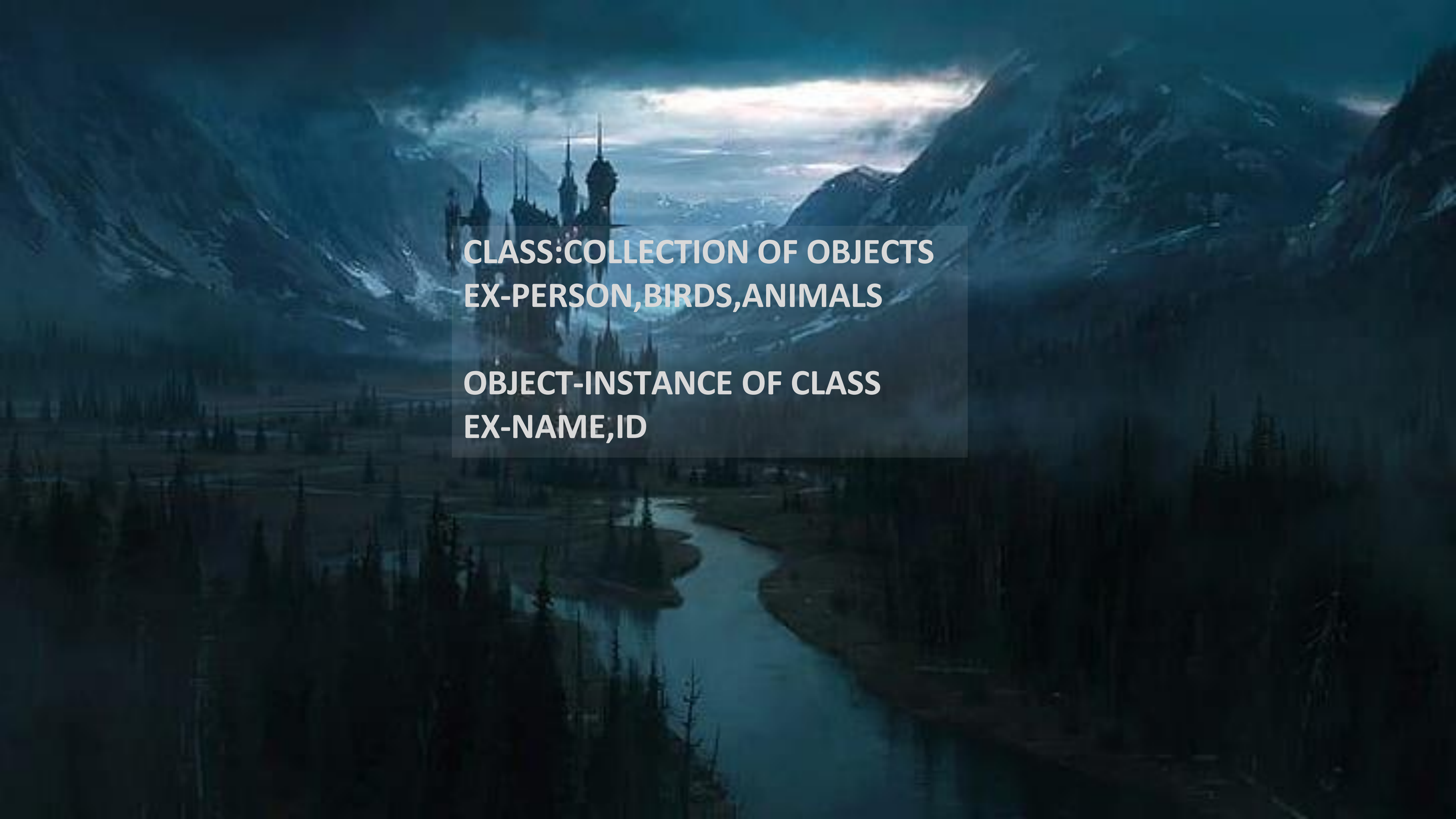
1
CLASS
OBJECT

2
ENCAPSULATION

3
ABSTRACTION

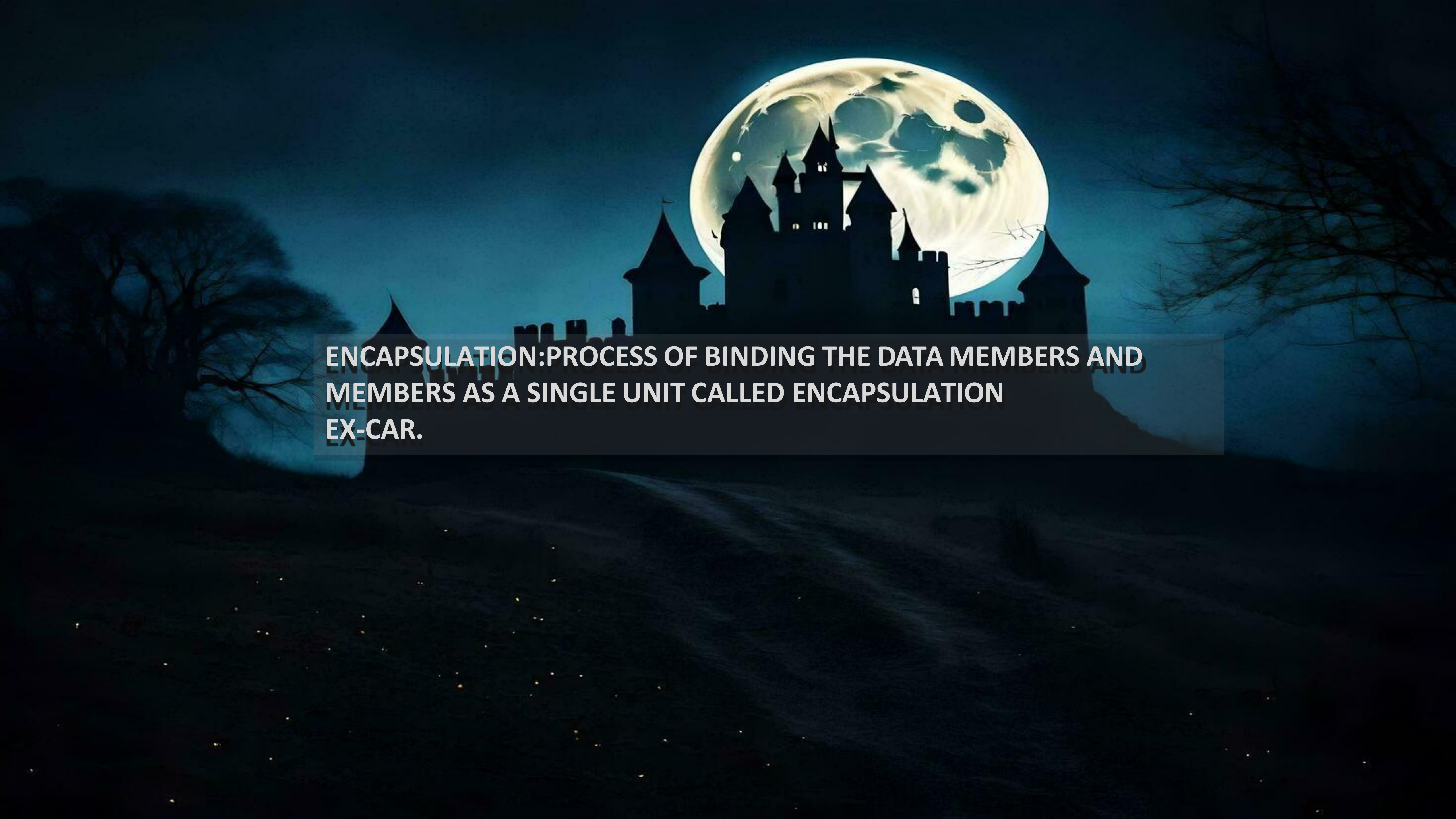
4
INHERITANCE

5
POLYMORPHISM



CLASS:COLLECTION OF OBJECTS
EX-PERSON,BIRDS,ANIMALS

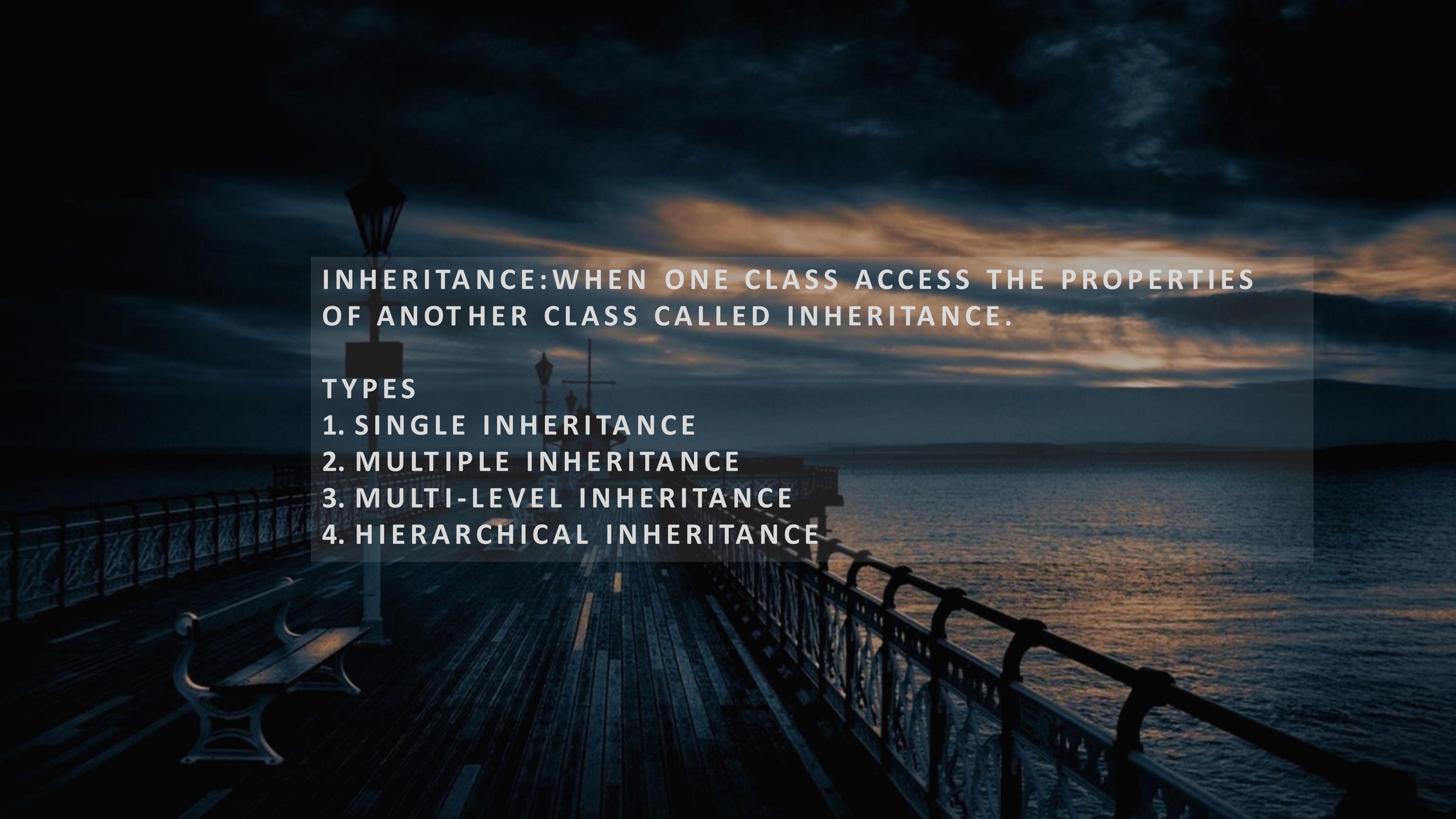
OBJECT-INSTANCE OF CLASS
EX-NAME,ID



ENCAPSULATION:PROCESS OF BINDING THE DATA MEMBERS AND MEMBERS AS A SINGLE UNIT CALLED ENCAPSULATION
EX-CAR.

ABSTRACTION:PROCESS IN WHICH INVOLVES HIDNING THE ESSENTIAL PART AND PROVIDING THE SET OF SERVICES CALLED ABSTRACTION.

EX-INTERNAL STRUCTER OF CAR HAVING BREAK BUT WE DON'T KNOW HOW IT ACTUALLY WORKS WHEN WE PUSH.



INHERITANCE:WHEN ONE CLASS ACCESS THE PROPERTIES OF ANOTHER CLASS CALLED INHERITANCE.

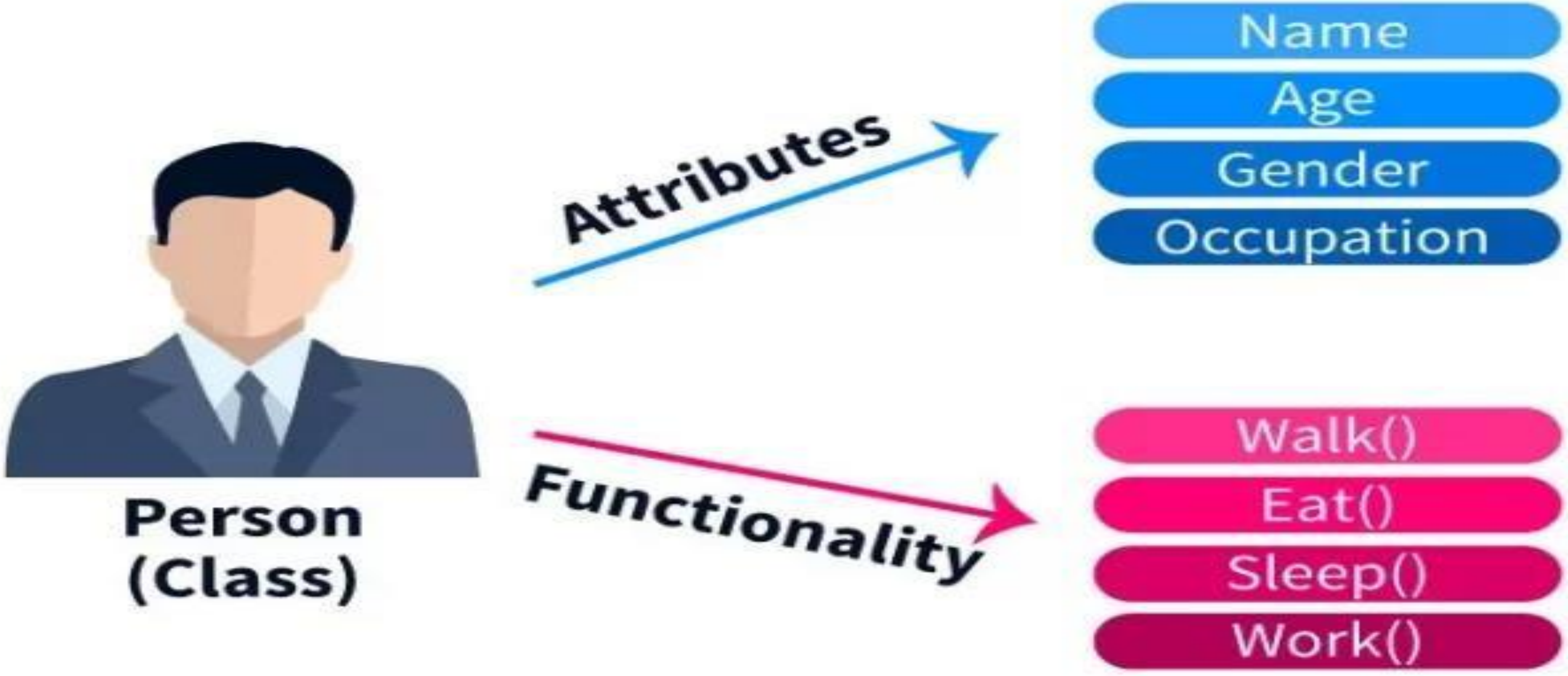
TYPES

1. SINGLE INHERITANCE
2. MULTIPLE INHERITANCE
3. MULTI-LEVEL INHERITANCE
4. HIERARCHICAL INHERITANCE

POLYMORPHISM:THE ACT OF REPRESENTING ONE FORM TO MANY FORMS .

TYPES OF POLYMORHISM:
1.COMPILETIME POLYMORPHISM
2.RUNTIME POLYMORPHISM

What is Class?



Person (Class)

Attributes

- Name
- Age
- Gender
- Occupation

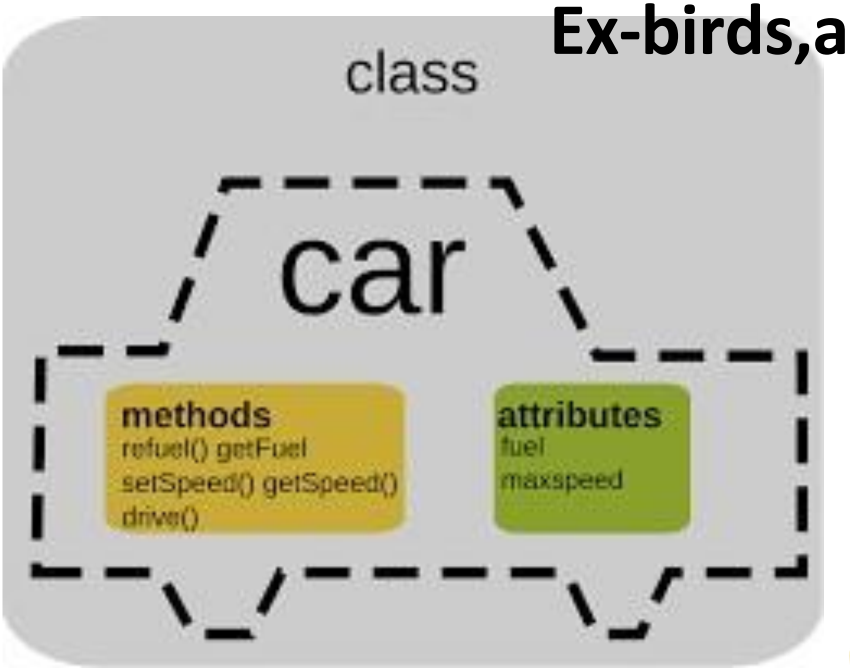
Functionality

- Walk()
- Eat()
- Sleep()
- Work()

SCALER Topics

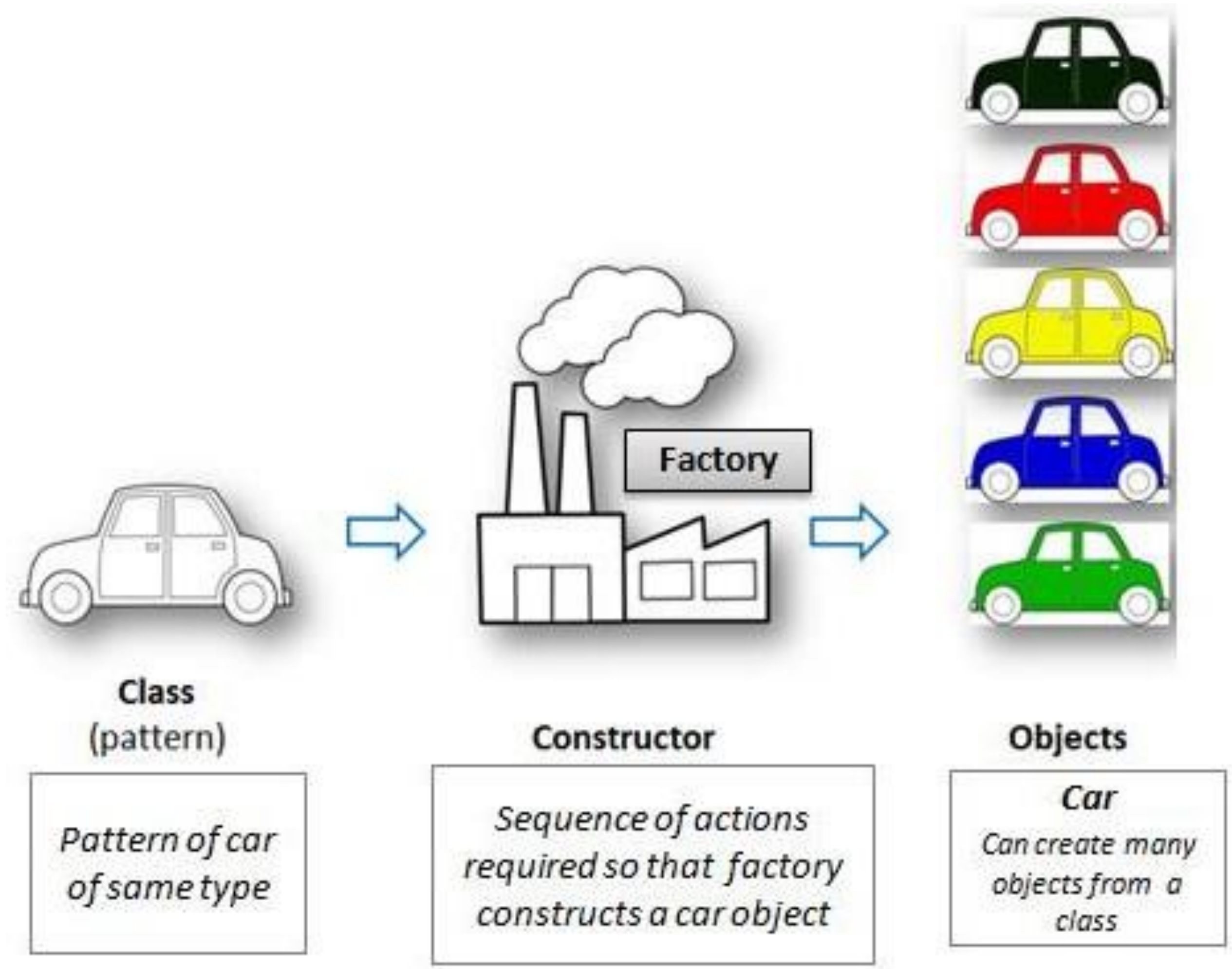
Class:-class is nothing but collection of Objects.

Ex-birds,animals,person.



Object:-object is instance of class

Ex-name,gender.



Class
(pattern)

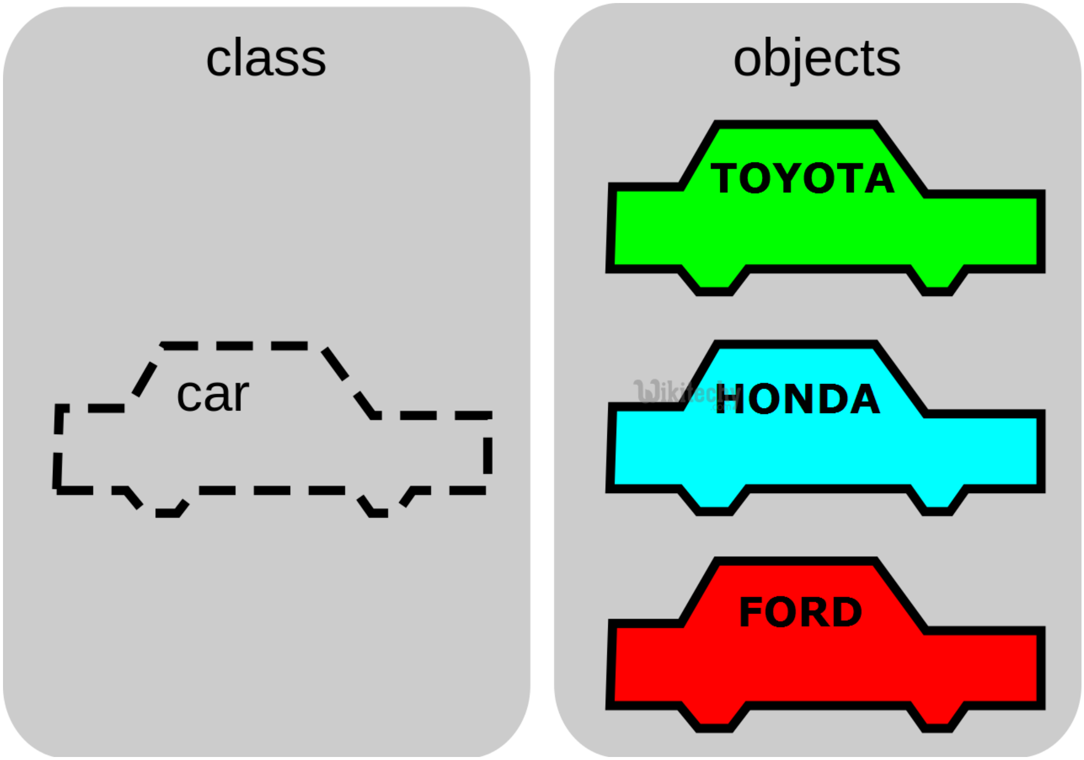
Pattern of car of same type

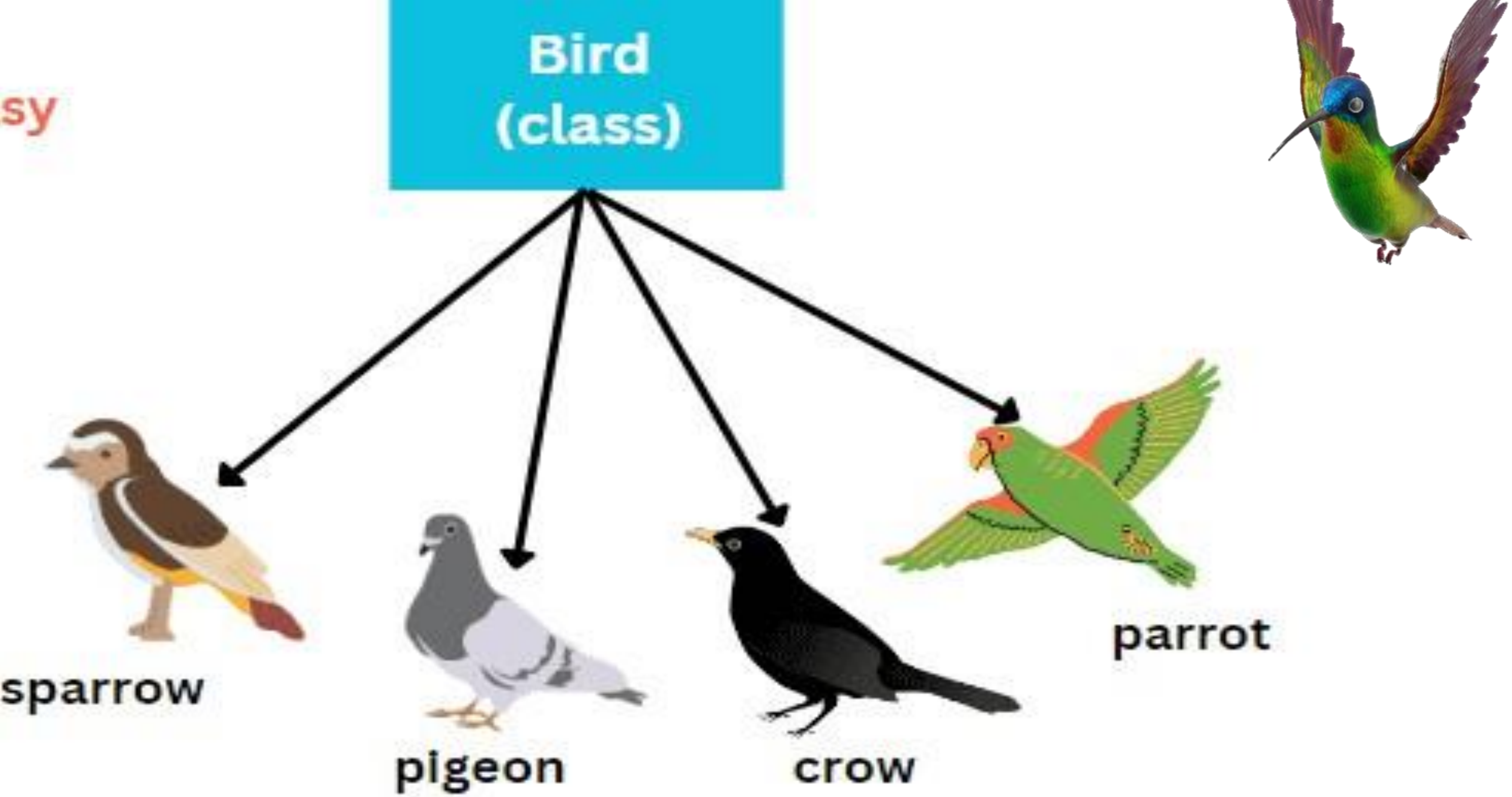
Constructor

Sequence of actions required so that factory constructs a car object

Objects

Car
Can create many objects from a class





Bird
(class)

sparrow

pigeon

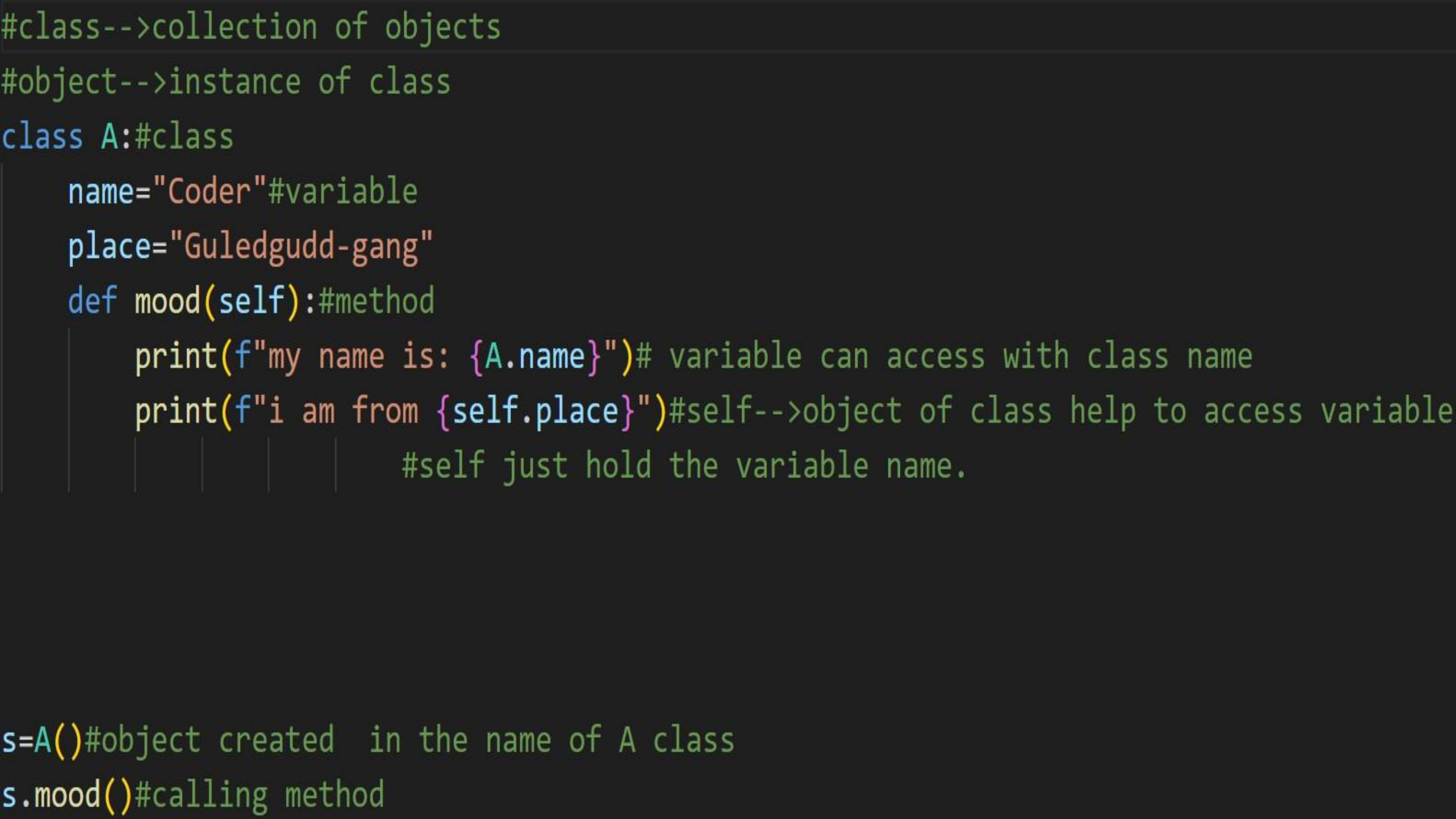
crow

parrot

Bird is a class and sparrow, pigeon, crow, parrot are objects of class Bird.

In Python or any other programming language, a class is a collection of as many as objects, which is common to all objects of one type.

Fig: Real-time examples of class and objects in Python



```
#class-->collection of objects
#object-->instance of class
class A:#class
    name="Coder"#variable
    place="Guledgudd-gang"
    def mood(self):#method
        print(f"my name is: {A.name}")# variable can access with class name
        print(f"i am from {self.place}")#self-->object of class help to access variable
                        #self just hold the variable name.




s=A()#object created  in the name of A class
s.mood()#calling method
```

CLASS AND OBJECT

DEMO PROGRAM:[CLICK HERE]

What is Encapsulation in Python?

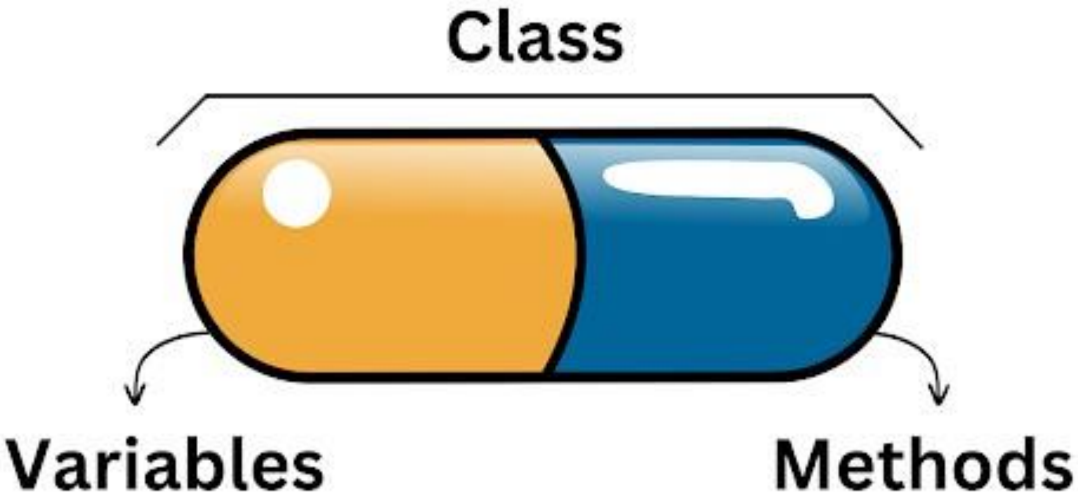
Class

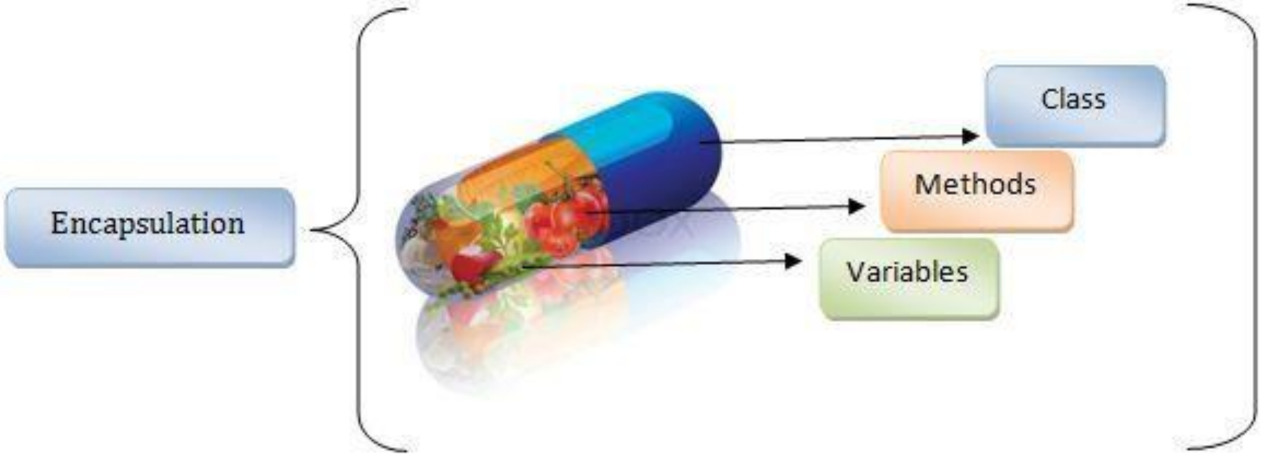
🟦 Variables

🟧 Methods

CODING NINJAS

ENCAPSULATION:THE PROCESS IN WHICH WE ARE GONNA BIND THE DATA MEMBERS(VARIABLES) AND MEMEBERS METHOD IN A SINGLE UNIT CALLED ENCAPSULATION.





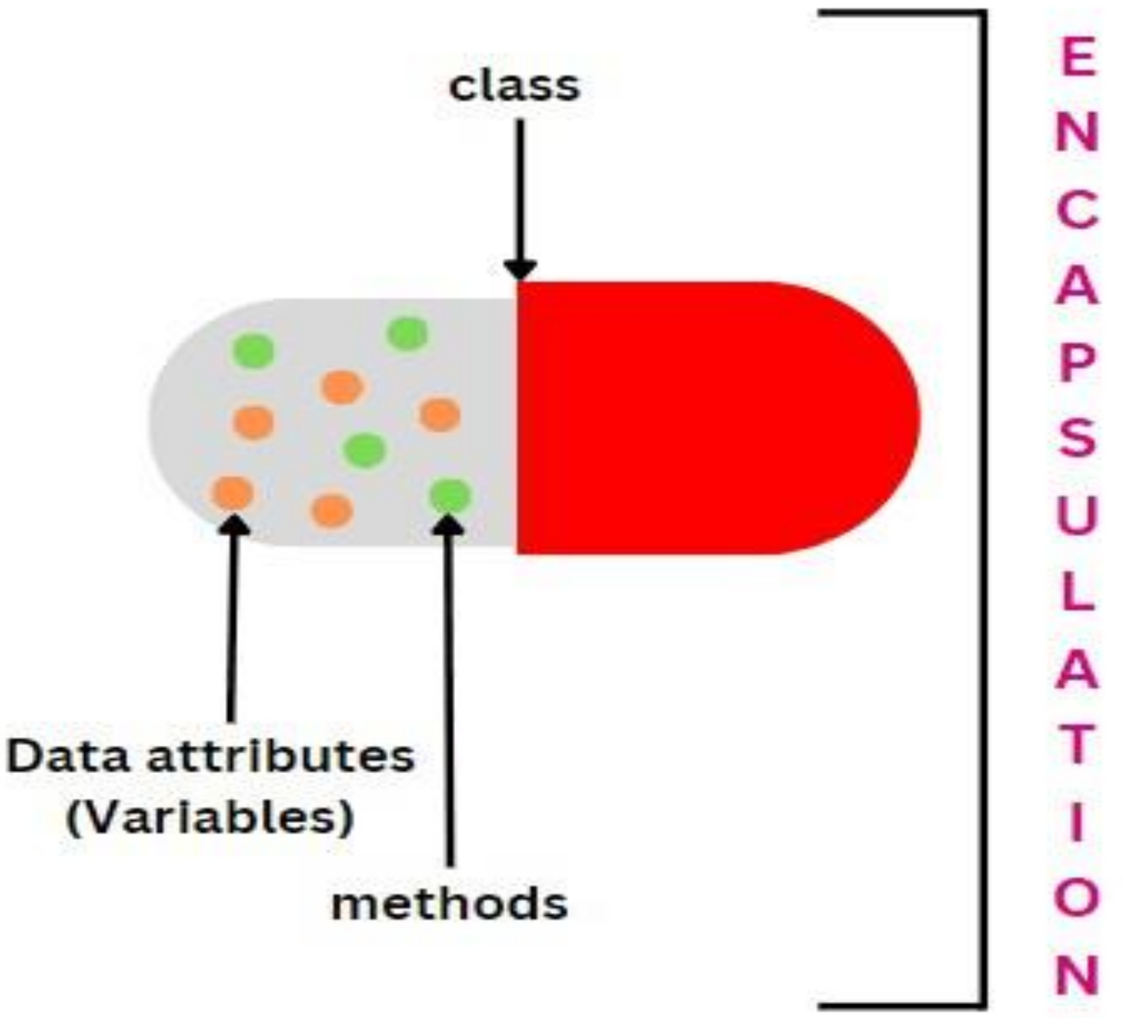
ENCAPSULATION

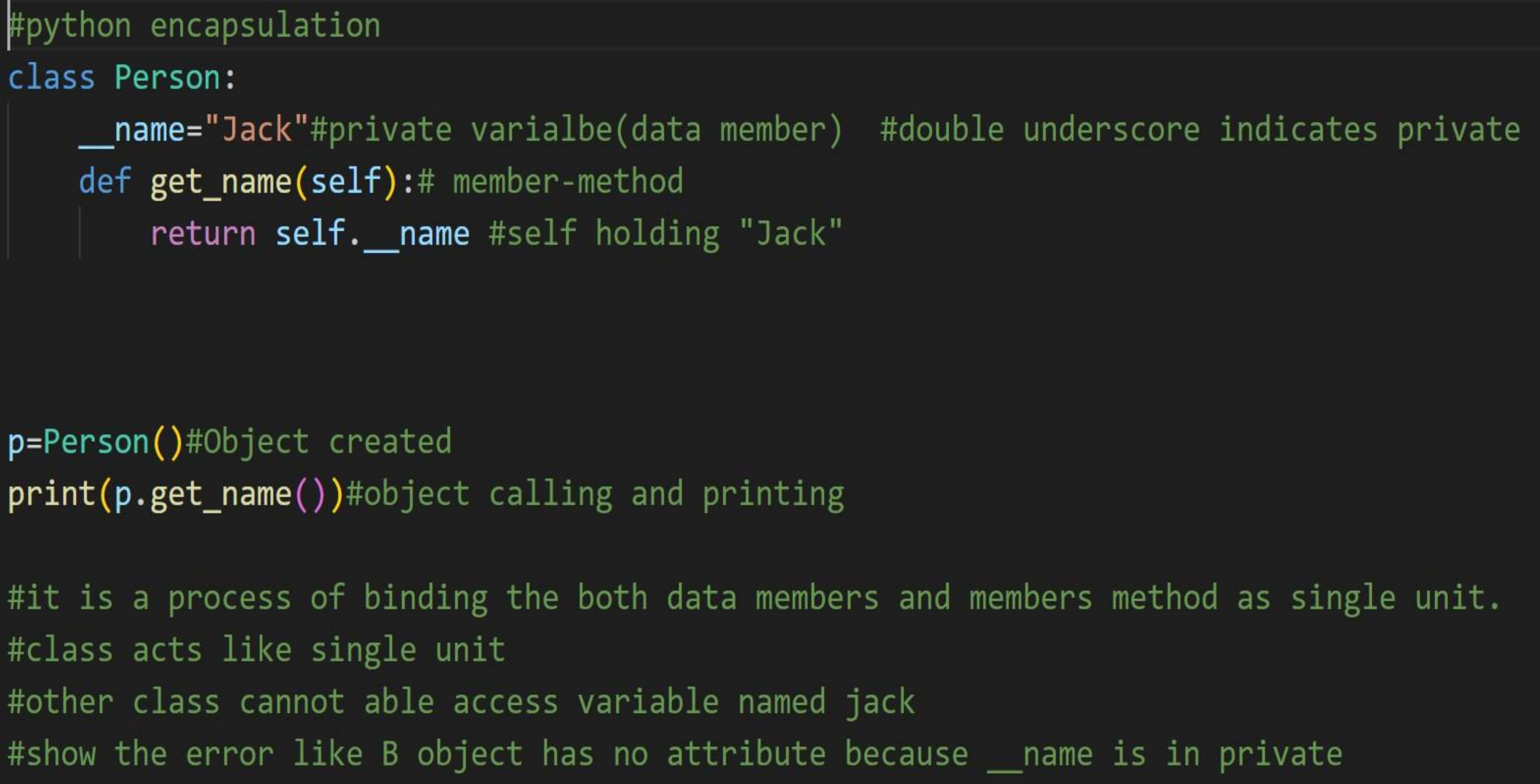
```
class Person:

    def __init__(self, name, age):

        self.name = name
        self.age = age

    def display(self):

        print(self.name)
        print(self.age)
```

Data attributes

Method

Wrapping up data and methods associated with that data into a single unit is called encapsulation in Python

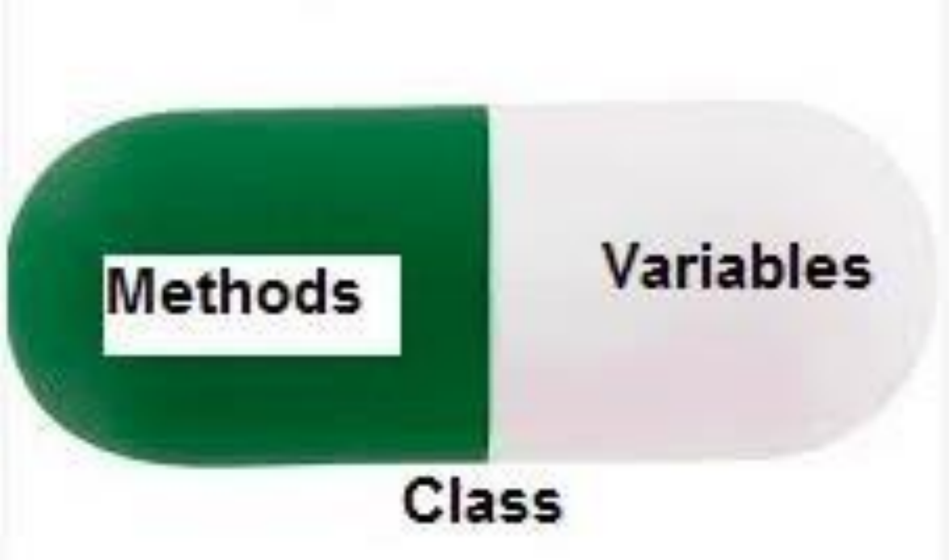




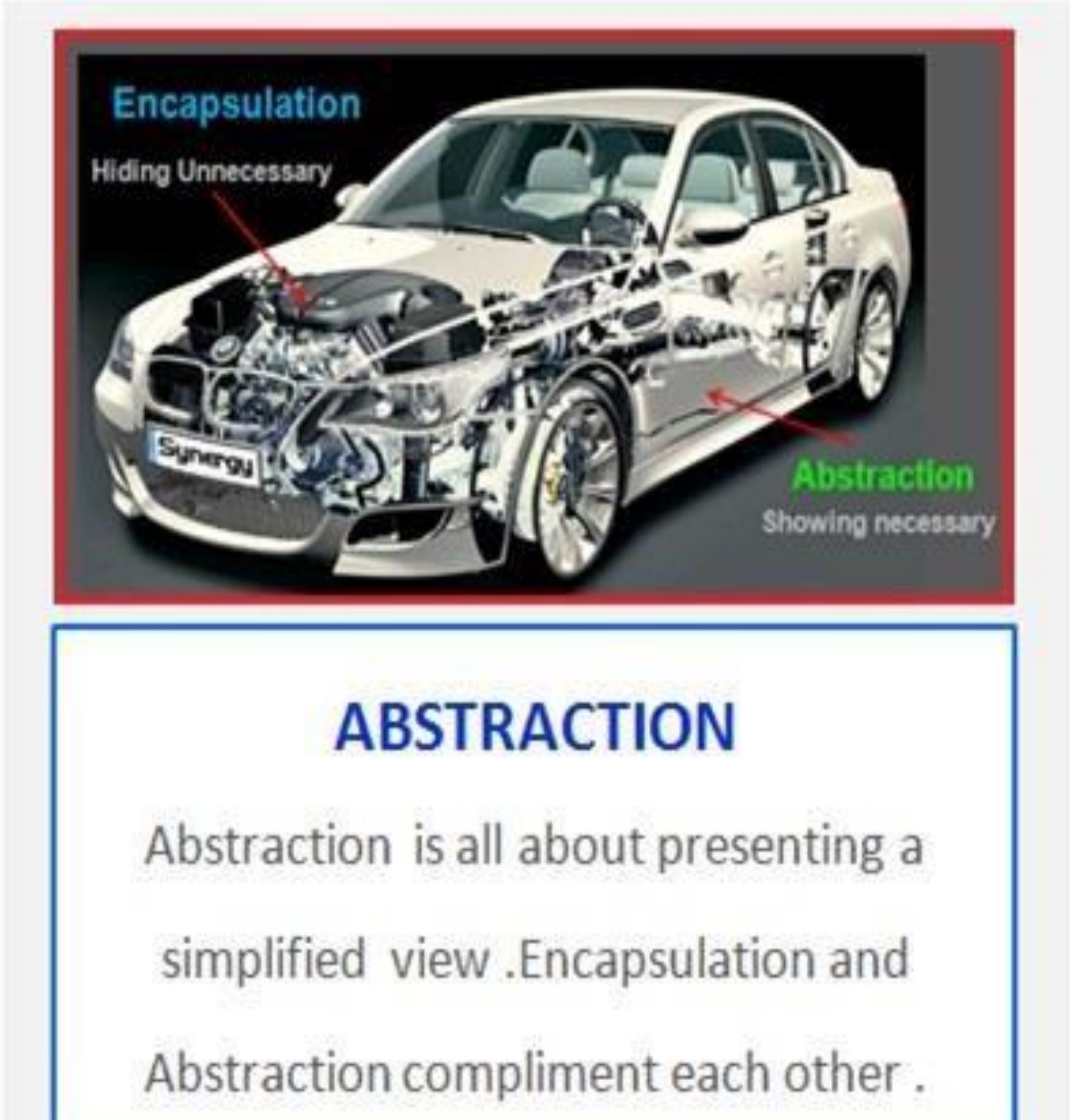
```python
#python encapsulation
class Person:
    __name="Jack"#private varialbe(data member)  #double underscore indicates private
    def get_name(self):# member-method
        return self.__name #self holding "Jack"



p=Person()#Object created
print(p.get_name())#object calling and printing

#it is a process of binding the both data members and members method as single unit.
#class acts like single unit
#other class cannot able access variable named jack
#show the error like B object has no attribute because __name is in private
```

ENCAPSULATION PROGRAM:-

DEMO PROGRAM:CLICK HERE



ABSTRACTION:



ABSTRACTION

Abstraction is all about presenting a simplified view .Encapsulation and Abstraction compliment each other .

ABSTRACTION:HIDING THE ESSENTIAL PART AND PROVIDING THE SET OF SERVICES CALLED ABSTRACTION.
EX-INTERNAL STRUCER OF CAR LIKE BREAK.

INTERFACES AND ABSTRACT CLASSES

THERE ARE TWO TYPES IN ABSTRACTION

1. ABSTRACT CLASS
2. INTERFACE CLASS

ABSTRACT CLASS:

ABSTRACT CLASS IS A TYPE OF CLASS WHICH CONTAINS BOTH ABSTRACT AND CONCRETE METHOD.

ABSTRACT METHOD:

TYPE OF METHOD WHICH HAS NO BODY.

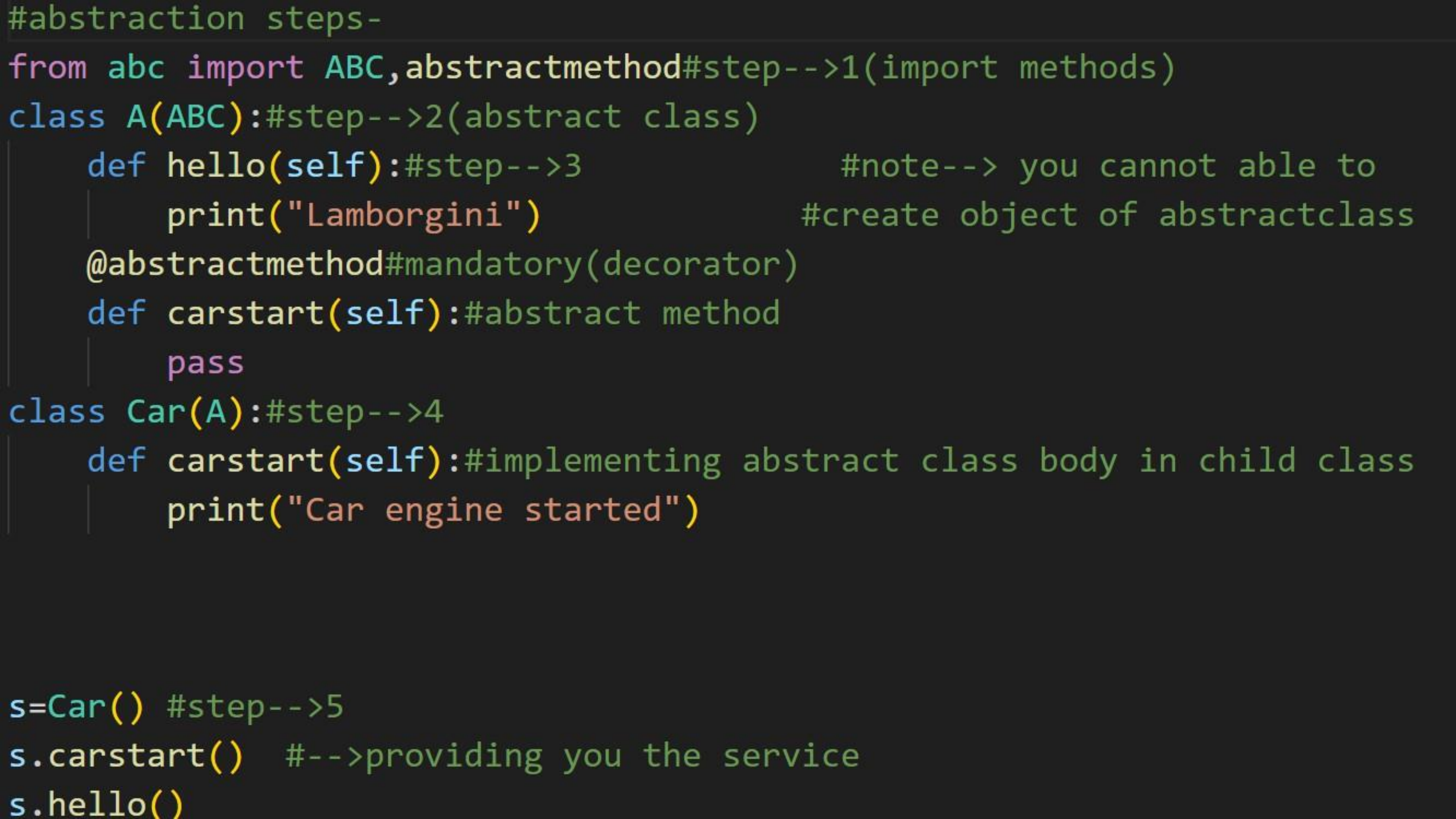
EX-
```
@abstractmethod
def sun(self):
    pass
```

CONCRETE METHOD:

TYPE OF METHOD WHICH HAS BODY

EX-
```
def hello(self):
    print(“Hello bro”)
    print(“How are you?”)
```


Using Abstraction
VS
Without Abstraction



```
#abstraction steps-
from abc import ABC,abstractmethod#step-->1(import methods)
class A(ABC):#step-->2(abstract class)
    def hello(self):#step-->3             #note--> you cannot able to
        print("Lamborgini")             #create object of abstractclass
    @abstractmethod#mandatory(decorator)
    def carstart(self):#abstract method
        pass
class Car(A):#step-->4
    def carstart(self):#implementing abstract class body in child class
        print("Car engine started")



s=Car() #step-->5
s.carstart()  #-->providing you the service
s.hello()
```

ABSTRACTION DEMO PROGRAM:

CLICK HERE

Interface in Python

INTERFACE CLASS

INTERFACE CLASS:TYPE OF A CLASS WHICH HAVING ONLY **ABSTRACT** METHOD CALLED INTERFACE CLASS, MEANS IMPLEMENTATION IS GOING TO DERIVE IN CHILD CLASS.

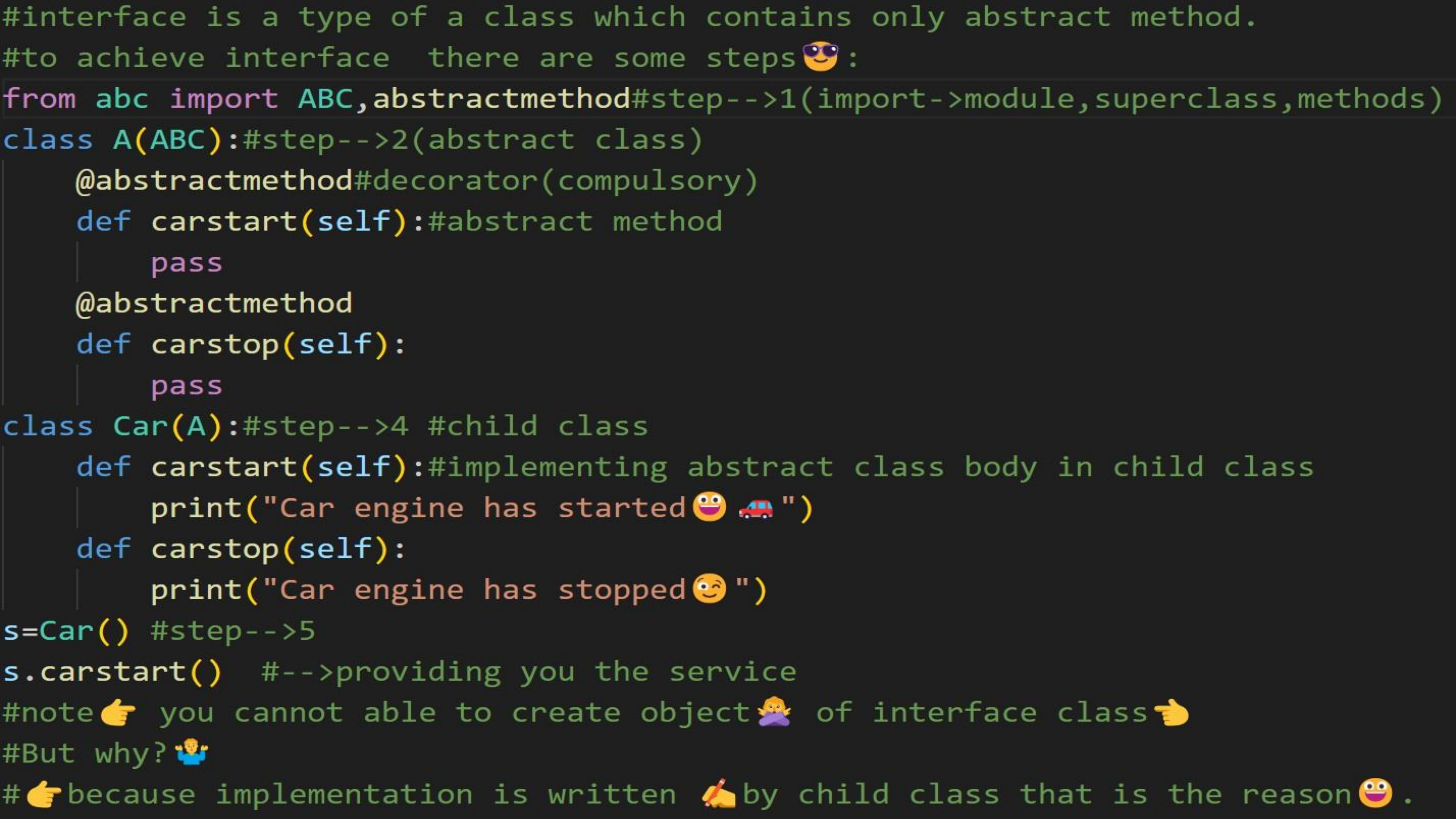
ABSTRACT METHOD:

THE METHOD WHICH HAS NO BODY
CALLED ABSTRACT METHOD.

```
EX-@abstractmethod
      def moon():
           pass
```

Python

Python how to Implement Interfaces

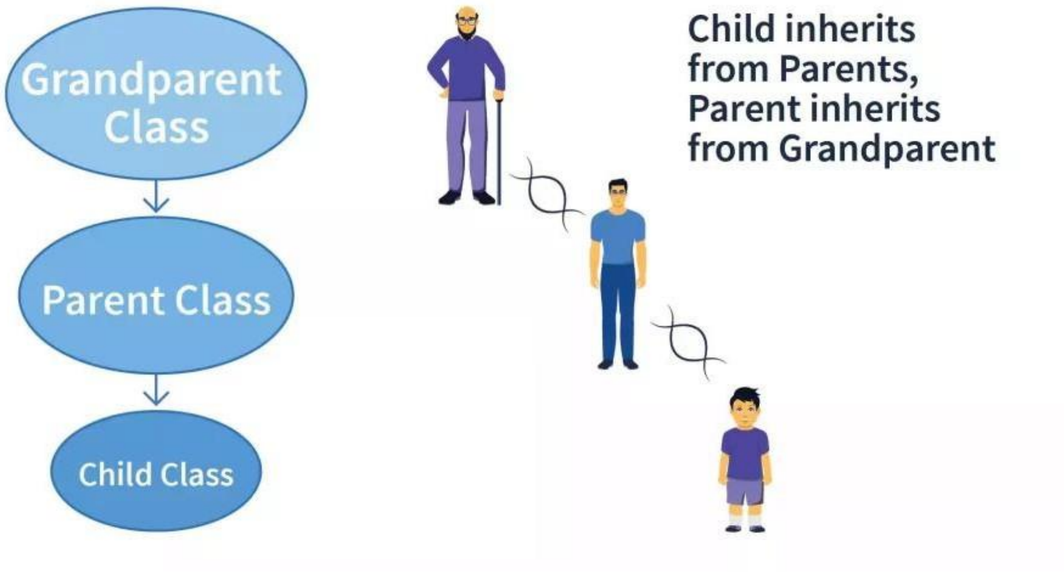


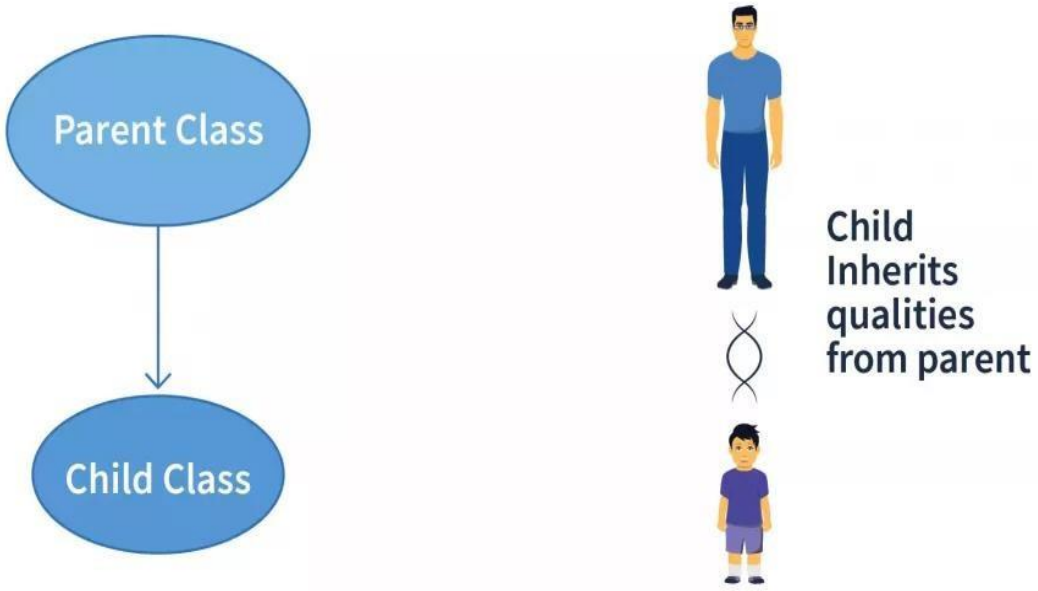
```
#interface is a type of a class which contains only abstract method.
#to achieve interface  there are some steps😎:
from abc import ABC,abstractmethod#step-->1(import->module,superclass,methods)
class A(ABC):#step-->2(abstract class)
    @abstractmethod#decorator(compulsory)
    def carstart(self):#abstract method
        pass
    @abstractmethod
    def carstop(self):
        pass
class Car(A):#step-->4 #child class
    def carstart(self):#implementing abstract class body in child class
        print("Car engine has started😃 🚗")
    def carstop(self):
        print("Car engine has stopped😉")
s=Car() #step-->5
s.carstart()  #-->providing you the service
#note👉 you cannot able to create object🙅 of interface class👉
#But why?🤷‍♂️
#👉because implementation is written ✍by child class that is the reason😃.
```

INTERFACE DEMO PROGRAM:

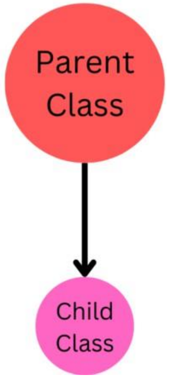
👉 CLICK HERE

INHERITANCE





INHERITANCE: WHEN CHILD CLASS ACCESS THE PROPERTIES FROM PARENT CLASS CALLED IT AS A INHERITANCE.



TYPES OF INHERITANCE:-

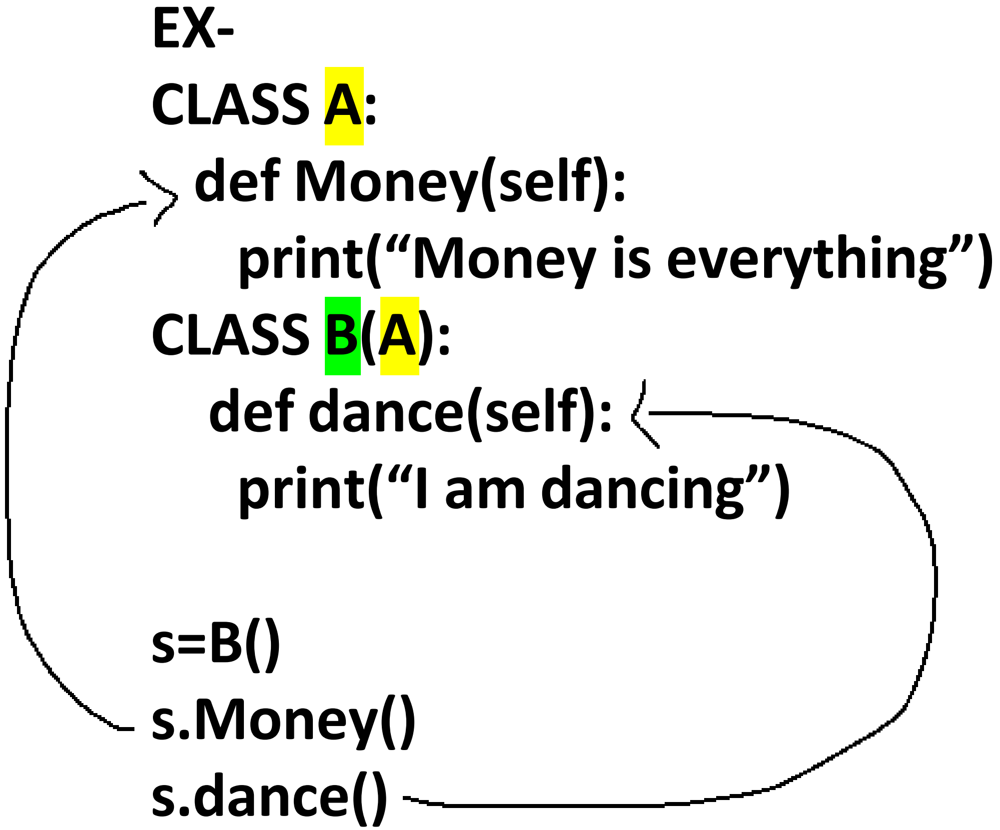
1. SINGLE INHERITANCE
2. MULTIPLE INHERITANCE
3. MULTI-LEVEL INHERITANCE
4. HIERARCHICAL INHERITANCE

SINGLE INHERITANCE:

IN SINGLE INHERITANCE THERE IS ONLY ONE PARENT CLASS AND ONLY ONE CHILD CLASS,AND CHILD CLASS IS GOING TO ACCESS THE PROPERTIES OF PARENT CLASS CALLED SINGLE INHERITANCE.

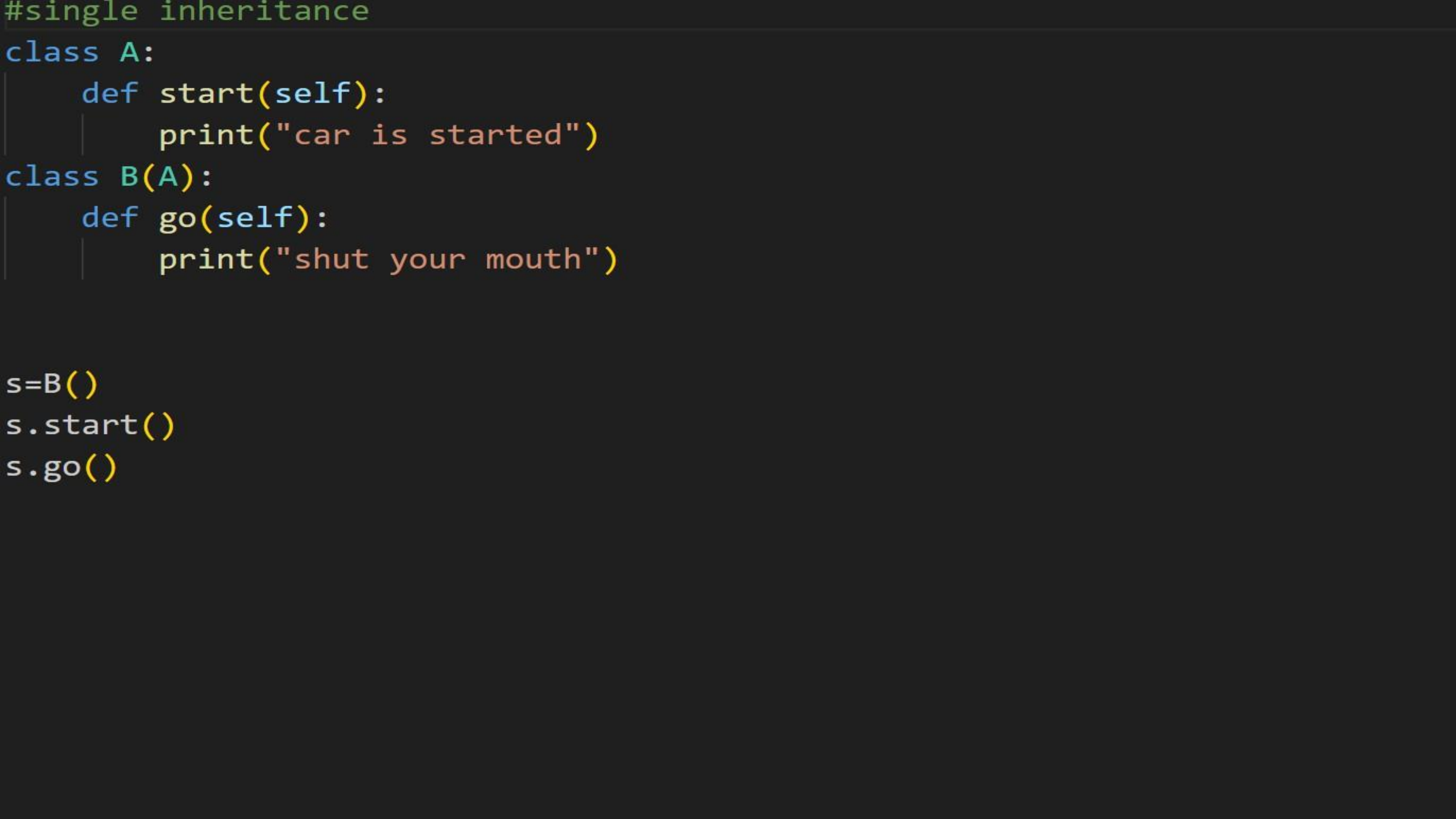
SYNTAX:

```
CLASS A:
  #METHOD
CLASS B(A):
  #METHOD
```



EX-

```
CLASS A:
  def Money(self):
     print(“Money is everything”)
CLASS B(A):
   def dance(self):
     print(“I am dancing”)

s=B()
s.Money()
s.dance()
```



```
#single inheritance
class A:
    def start(self):
        print("car is started")
class B(A):
    def go(self):
        print("shut your mouth")


s=B()
s.start()
s.go()
```

DEMO PROGRAM OF SINGLE INHERITANCE:

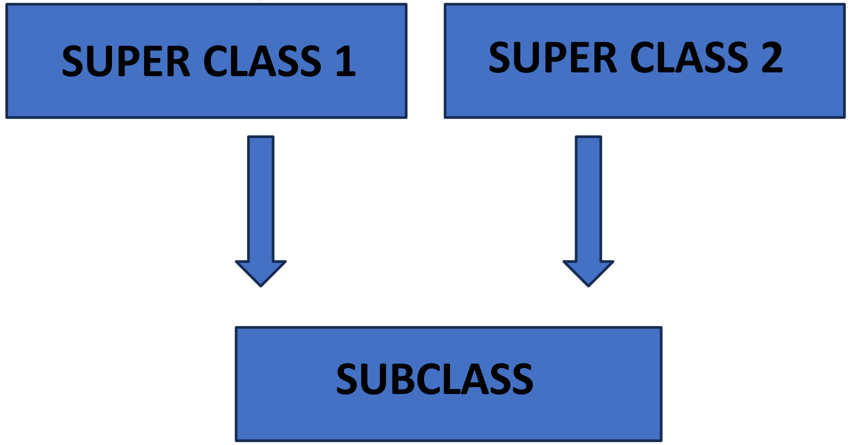
CLICK HERE:

MULTIPLE INHERITANCE

WHEN CHILD CLASS IS DERVIED BY TWO OR MORE SUPER CLASS THEN IT IS CALLED MULTIPLE INHERITANCE.

SYNTAX

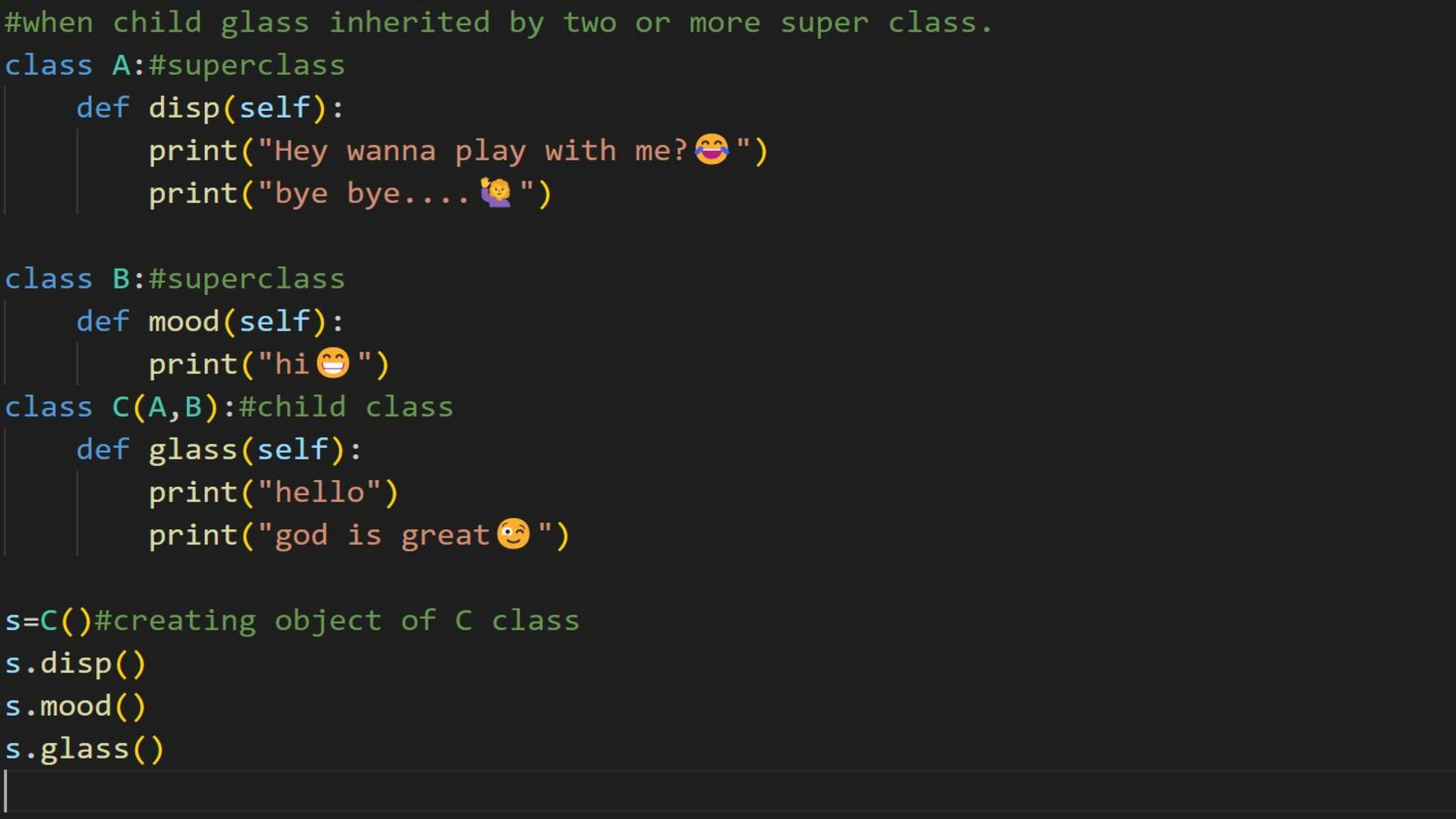
```
CLASS A:

  #METHOD

CLASS B:
  #METHOD

CLASS C(A,B):
   #METHOD
```



SUPER CLASS 1

SUPER CLASS 2

SUBCLASS



```python
#when child glass inherited by two or more super class.
class A:#superclass
    def disp(self):
        print("Hey wanna play with me?😂")
        print("bye bye....🙋‍♀️")

class B:#superclass
    def mood(self):
        print("hi😁")
class C(A,B):#child class
    def glass(self):
        print("hello")
        print("god is great😉")

s=C()#creating object of C class
s.disp()
s.mood()
s.glass()
```

DEMO PROGRAM OF MULTIPLE INHERITANCE:

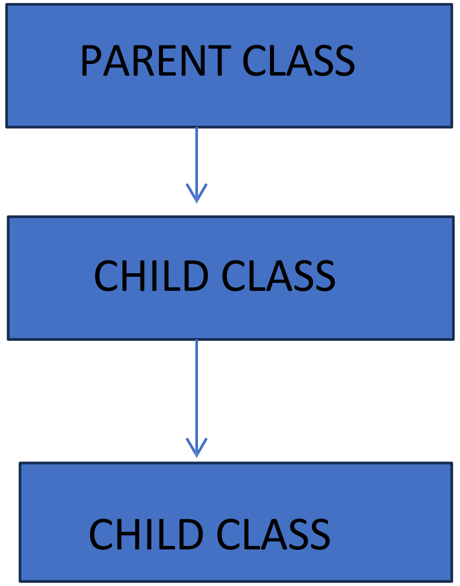
CLICK HERE:

MULTILEVEL-INHERITANCE:

IN THIS INHERITANCE WE HAVE ONLY ONE PARENT CLASS AND MULTIPLE CHILD CLASS

SYNTAX:

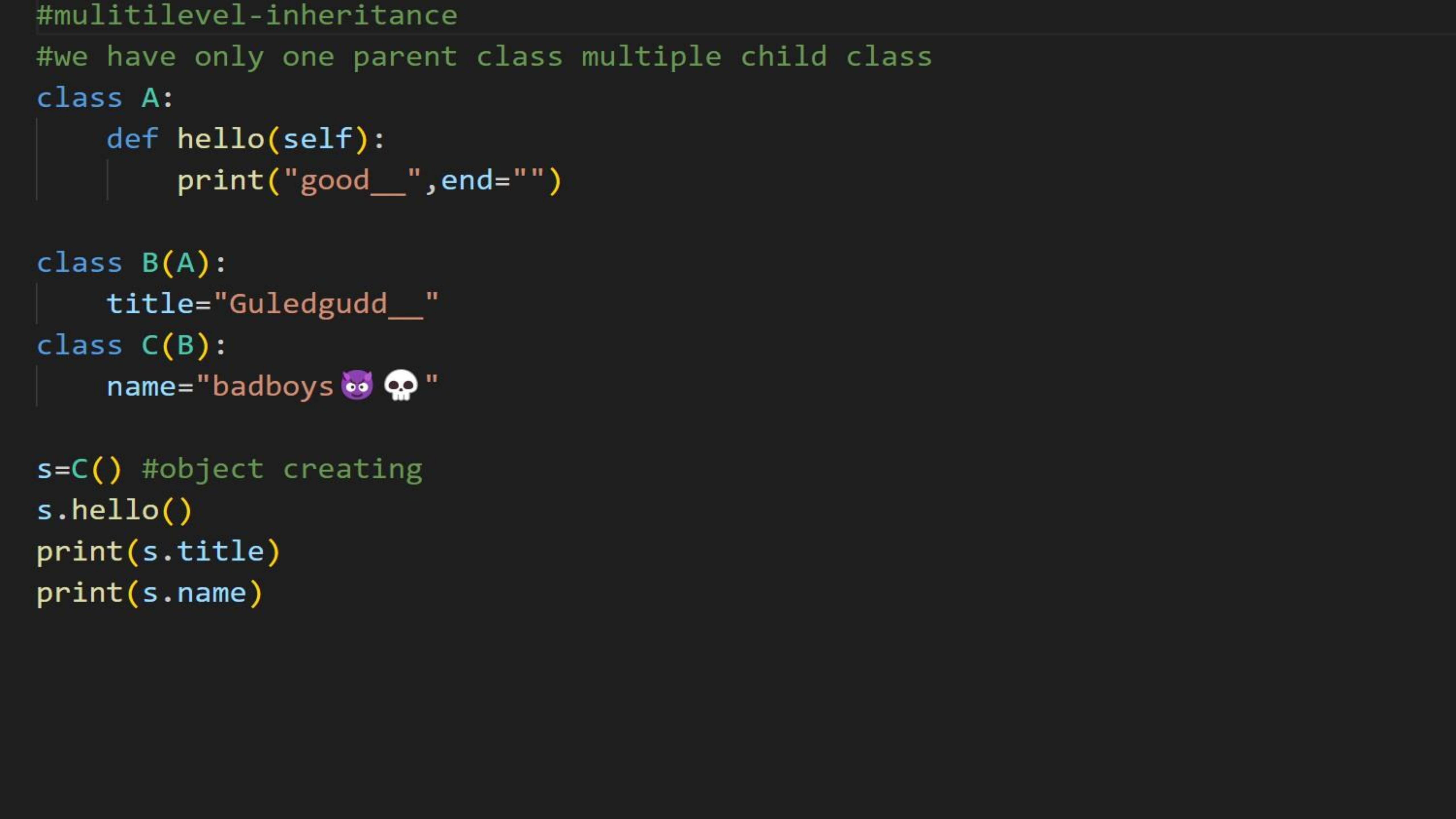
```
CLASS A:
 #MEHTOD

CLASS B(A):
 #MEHTOD

CLASS C(B)
 #METHOD
```



PARENT CLASS

CHILD CLASS

CHILD CLASS



```
#mulitilevel-inheritance
#we have only one parent class multiple child class
class A:
    def hello(self):
        print("good__",end="")

class B(A):
    title="Guledgudd__"
class C(B):
    name="badboys😈💀"

s=C() #object creating
s.hello()
print(s.title)
print(s.name)
```

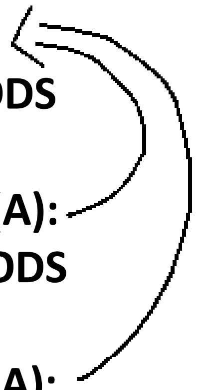
DEMO PROGRAM OF MULTI-LEVEL INHERITANCE:

👉CLICK HERE:

HIERARCHICAL –INHERITANCE:

IN THIS INHERITANCE THERE IS ONLY ONE **PARENT CLASS** AND **MULTIPLE CHILD CLASS** AND EACH CHILD CLASS DIRECTLY ACCESS THE PARENT CLASS .

SYNTAX:-



```
CLASS A:
#METHODS

CLASS B(A):
 #METHODS

CLASS C(A):
 #METHODS
```

DEMO PROGRAM OF HIERARCHICAL INHERITANCE:

👉CLICK HERE

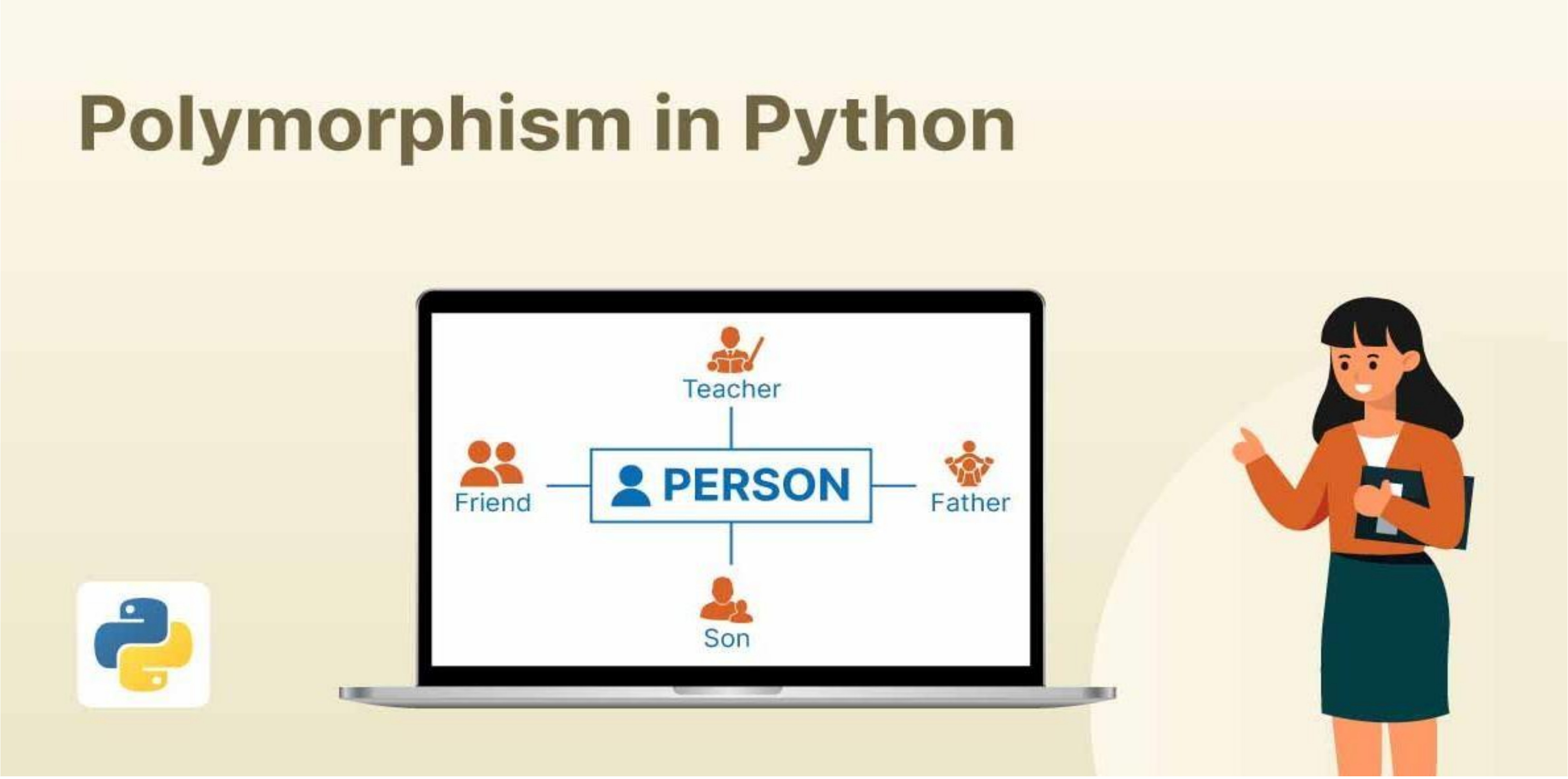
Polymorphism in Python

POLYMORPHISM:

THE ACT OF REPRESENTING ONE FORM TO MANY FORMS CALLED POLYMORPHISM.

#THERE ARE TWO TYPES IN POLYMORPHISM:-

1 .COMPILE TIME POLYMORPHISM(METHOD OVERLOADING)
2.RUNTIME POLYMORPHISM(METHOD OVERRIDING)



METHOD OVERLOADING(COMPILE TIME POLYMORPHISM)

WHENEVER A CLASS CONTAIN MORE THAN ONE METHOD HAVING SAME NAME WITH DIFFERENT PARAMETERS CALLED METHOD OVERLOADING.

SYNTAX:

```
CLASS A:
  def  method1(self):
       #code
  def method1(self,parameter1):
      #code
  def method1(self,parameter2,parameter3):
      #code
```

METHOD OVERRIDING(RUNTIME POLYMORPHISM)

WHEN WE DEFINE METHOD IN PARENT CLASS AND CHILD CLASS HAVING SAME METHOD NAME AND SAME PARAMETERS CALLED OVERRIDING.

SYNTAX:

```
CLASS A:
   def disp(self,parameter1):
      #code
CLASS B:
 def disp(self,parameter1):
      #code
```

References:

https://youtube.com/playlist?list=PLqleLpAMfxGD-KFajIKzH24p6bgG5R_aN&si=qk4TcfiWwKFtGhFR

B.V.V.S Sangh's
BASAVESHWAR SCIENCE COLLEGE BAGALKOT
DEPARTMENT OF CHEMISTRY

Semester: B.Sc-VI Semester **Subject: Chemistry**
Unit: TERPENOIDS **Name: Dr. D. S. Lamani**
Course Code: 21BSC6C6 CHE8L

Dr. DSL

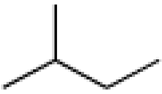
TERPENOIDS

Terpenes and Terpenoids constitute a large class of natural products built up from Classification, General methods of extraction and separation (Mono and sesquiterpenes), special isoprene rule and Structural elucidation of citral, carvone, menthol & camphor isoprene units. Terpenes are technically only hydrocarbons, while terpenoids are oxygenated.

Isoprene Rule:

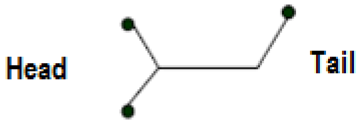
- The basic molecular formulae of terpenes are multiples of **$(C_5H_8)_n$** where n is the number of linked isoprene units.

Isoprene

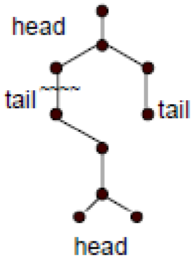


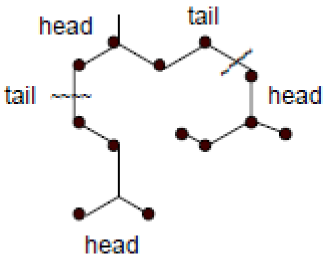
Isoprene Unit

- Isoprene rule stats that the terpenoid molecules are constructed from two or more isoprene unit.
- Further Ingold suggested that isoprene units are joined in the terpenoid via 'head to tail' fashion.
- Special isoprene rule states that the terpenoid molecules are constructed of two or more isoprene units joined in a **'head to tail'** fashion.

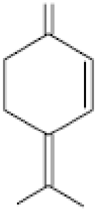


- But this rule can only be used as guiding principle and not as a fixed rule. For example carotenoids are joined tail to tail at their central and there are also some terpenoids whose carbon content is not a multiple of five.
- In applying isoprene rule we look only for the skeletal unit of carbon. The carbon skeletons of open chain monotrpenoids and sesqui terpenoids are,

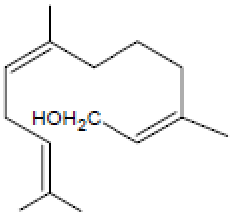




Examples.

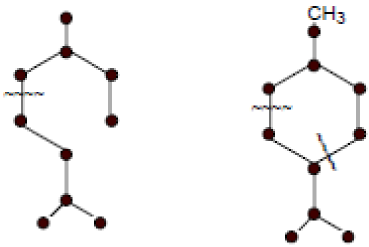


Myrcene (*Monoterpene*)



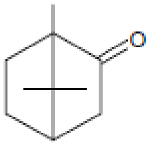
Farnesol (*Sesquiterpene*)

- Ingold (1921) pointed that a gem alkyl group affects the stability of terpenoids. He summarized these results in the form of a rule called 'gem dialkyl rule' which may be stated as "Gem dialkyl group tends to render the cyclohexane ring unstable where as it stabilizes the three, four and five member rings."
- This rule limits the number of possible structure in closing the open chain to ring structure.Thus the monoterpenoid open chain give rise to only one possibility for a monocyclic monoterpenoid i.e the p-cymene structure.

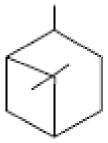


P-cymene structure

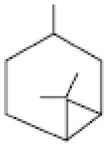
- Bicyclic monoterpenodis contain a six member and a three member ring. Thus closure of the ten carbon open chain monoterpenoid gives three possible bicyclic structures.



Camphor
(6+5) system



Pinane
(6+4) system



Carane
(6+3) System

CLASSIFICATION OF TERPENOIDS

Most natural terpenoid hydrocarbon have the general formula (C5H8)n. They can be classified on the basis of value of n or number of carbon atoms present in the structure.

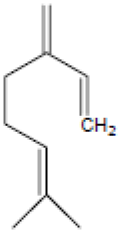
S.No.	Number of carbon atoms	Value of n	Class
1	10	2	Monoterpenoids ($C_{10}H_{16}$)
2	15	3	Sesquiterpenoinds ($C_{15}H_{24}$)
3	20	4	Diterpenoids ($C_{20}H_{32}$)
4	25	5	Sesterpenoids ($C_{25}H_{40}$)
5	30	6	Troterpenoids ($C_{30}H_{48}$)
6	40	8	Tetraterpinoid ($C_{40} H_{64}$)
7	>40	>8	Polyterpinoids ($(C_5 H_8)_n$)

Each class can be further subdivided into subclasses according to the number of rings present in the structure.

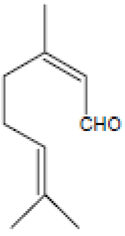
I. **Acyclic Terpenoids**: They contain open structure.
II. **Monocyclic Terpenoids:** They contain one ring in the structure.
III. **Bicyclic Terpenoids:** They contain two rings in the structure.
IV. **Tricyclic Terpenoids:** They contain three rings in the structure.
V. **Tetracyclic Terpenoids:** They contain four rings in the structure.

A) Mono Terpenoids:

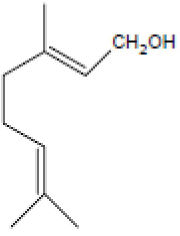
i) Acyclic Monoterpenoids



Myrcene

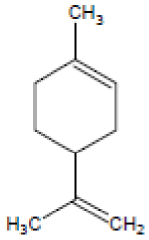


Citral

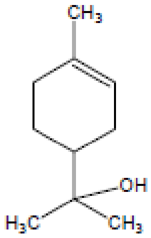


Geraniol

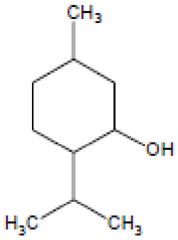
ii) *Monocyclic monoterpenoids*



Limonene



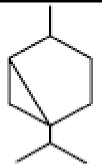
α-Terpineol



Menthol

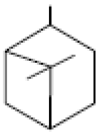
iii) *Bicyclic monoterpenoids:* These are further divided into three classes.

- Containing -6+3 membered rings



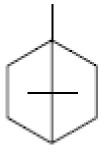
Thujane

- Containing 6+4 membered rings



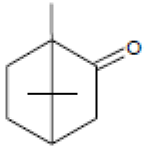
Pinane

- Containing 6+5 membered rings

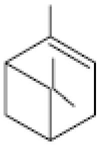


Bormane (Camphane)

- Some bicyclic monoterpenes are



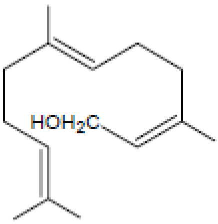
Camphor



alfa-pinene

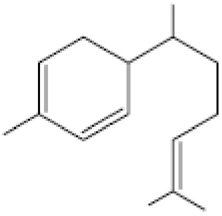
B) Sesquiterpenoids:

i) *Acyclic sesquiterpenoids*



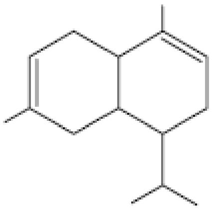
Farnesol

ii) *Monocyclic sesquiterpenoids*



Zinziberene

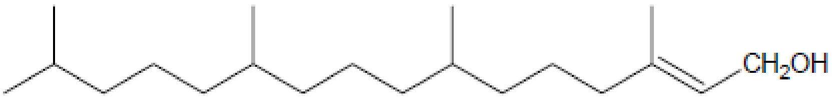
iii) *Bicyclic sesquiterpenoids*.



Cadinene

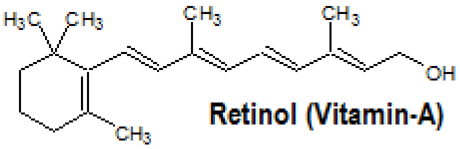
C) Diterpenoids:

i) Acyclic diterpenoids

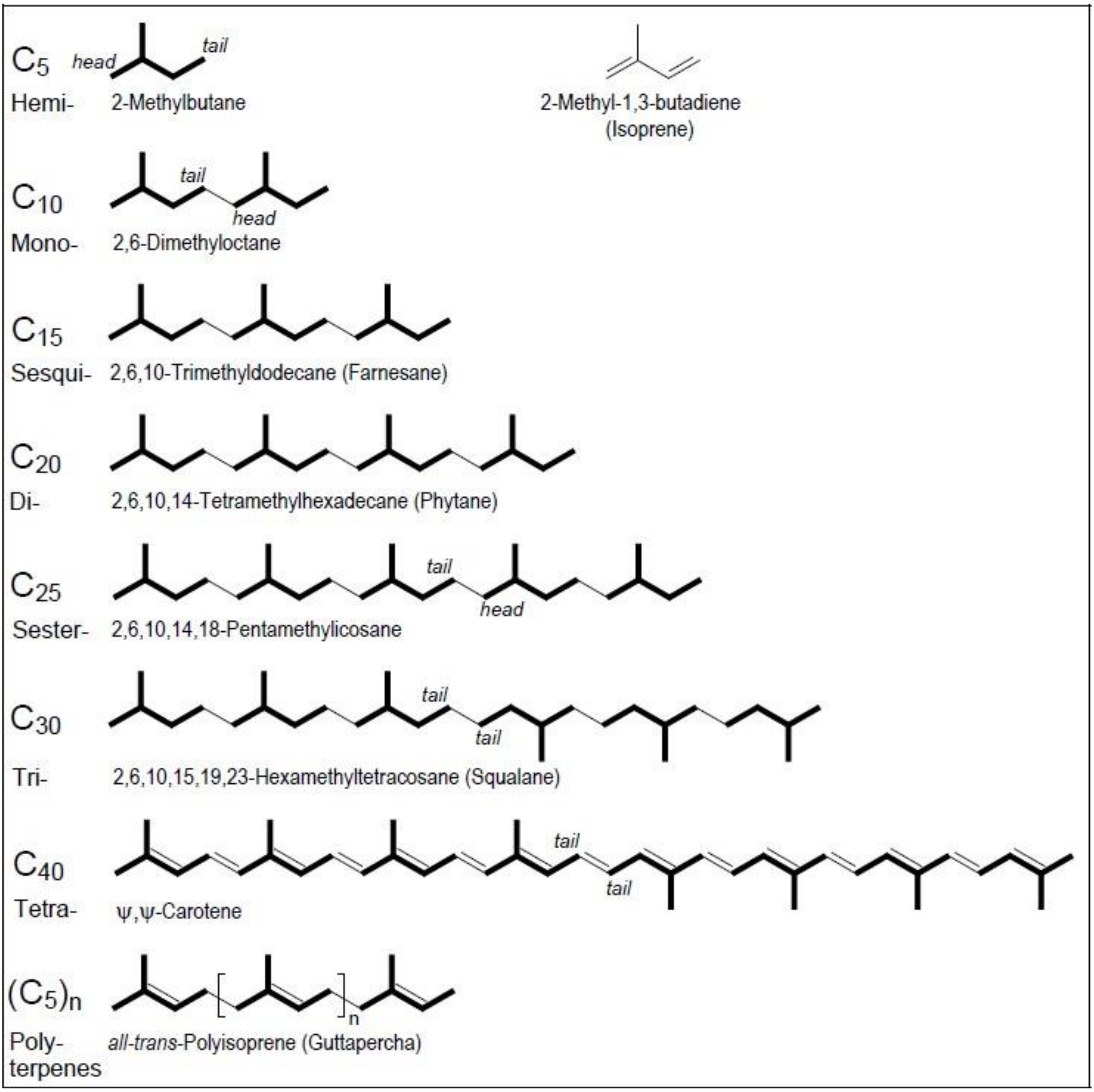


Phytol

ii) Mono cyclic diterpenoids:

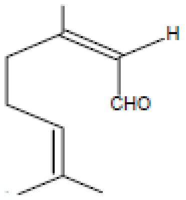


Retinol (Vitamin-A)

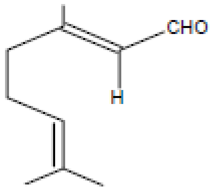

C5
head
tail
Hemi-
2-Methylbutane
2-Methyl-1,3-butadiene
(Isoprene)
C10
tail
head
Mono-
2,6-Dimethyloctane
C15
Sesqui-
2,6,10-Trimethyldodecane (Farnesane)
C20
Di-
2,6,10,14-Tetramethylhexadecane (Phytane)
C25
tail
head
Sester-
2,6,10,14,18-Pentamethylicosane
C30
tail
tail
Tri-
2,6,10,15,19,23-Hexamethyltetracosane (Squalane)
C40
tail
tail
Tetra-
ψ,ψ-Carotene
(C5)n
n
Poly-
terpenes
all-trans-Polyisoprene (Guttapercha)

CITRAL:

- Citral is an acyclic monoterpenoid. It is a major constituent of lemon grass oil in which it occurs to an extent of 60-80%.
- It is pale yellow liquid having strong lemon like odour, boiling point 224-228° C and can be obtained by fractional distillation under reduced pressure from Lemongrass oil.
- _Isomerism of citral_: Two geometrical isomers occur in nature. The ***cis*-isomers** is known as **Citral-a** and ***trans*-isomers Citral-b**.
- Ordinary citral obtained from lemongrass oil is, in fact, mixture of **Citral-a (90%)** and **Citral-b (10%)**.



Cis-citral; citral-b: neral; Z-form

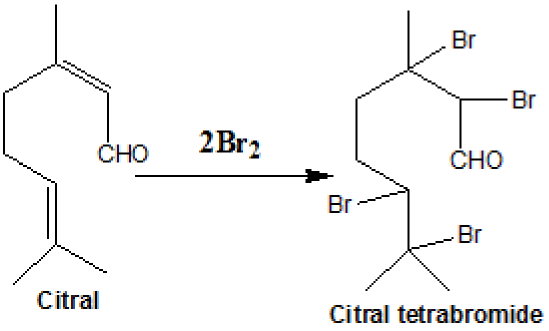


Trans-citral; Citral-a; geranial; E-form

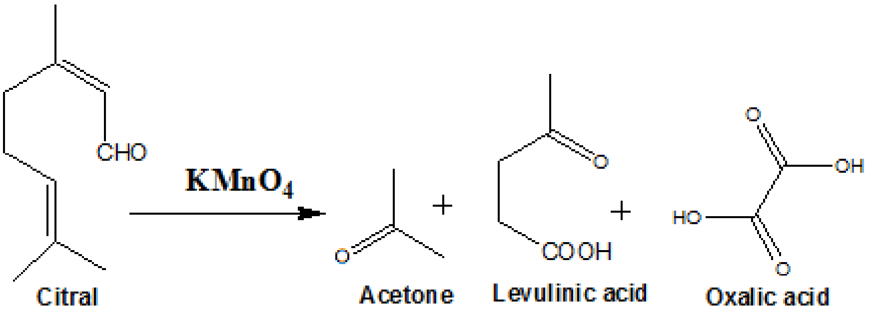
- **Uses:** It is extensively used in perfume and flavour industry and manufactures of vitamin A. Recently it become as a drug for reducing blood pressure.

STRUCTURE ELUCIDATION

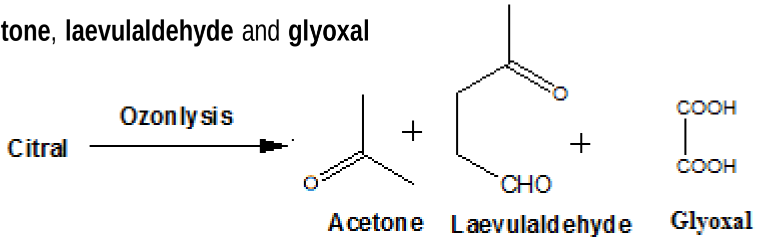
- ➢ Mol formula was determined as $C_{10}H_{16}O$
- ➢ Presence of two C=C: It adds two molecules of bromine to form a tetrabromide, which indicate the presence of two carbon-carbon double bonds.



- ➢ _Position of C=C bonds indicate_: Oxidation of citral with alkaline $KMnO_4$, gives **Acetone**, **Levulinic acid** and **Oxalic acid**.

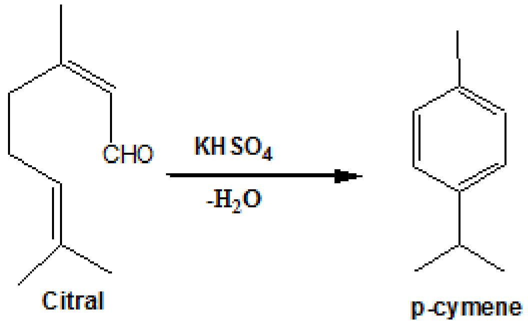


- *On ozonlysis*: It gives **acetone**, **laevulaldehyde** and **glyoxal**

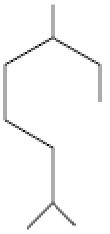


Formation of above products shows that citral is an acyclic compound containing two double bonds. Corresponding saturated hydrocarbon of citral (mol. Formula $C_{10}H_{22}$) corresponds to the general formula C_nH_{2n+2} for acyclic compounds, indicating that citral must be an acyclic compound.

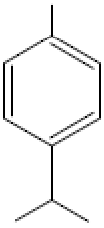
- Formation of p-cymene and product obtained from the ozonolysis reveals that citral is formed by the joining of two isoprene units in the head to tail fashion.



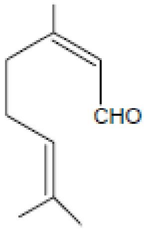
- On the basis of above facts following structure were proposed for citral.



Carbon skelton of citral

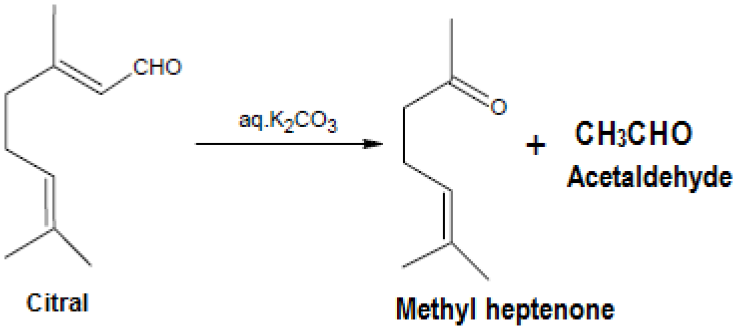


p-cymene



Citral

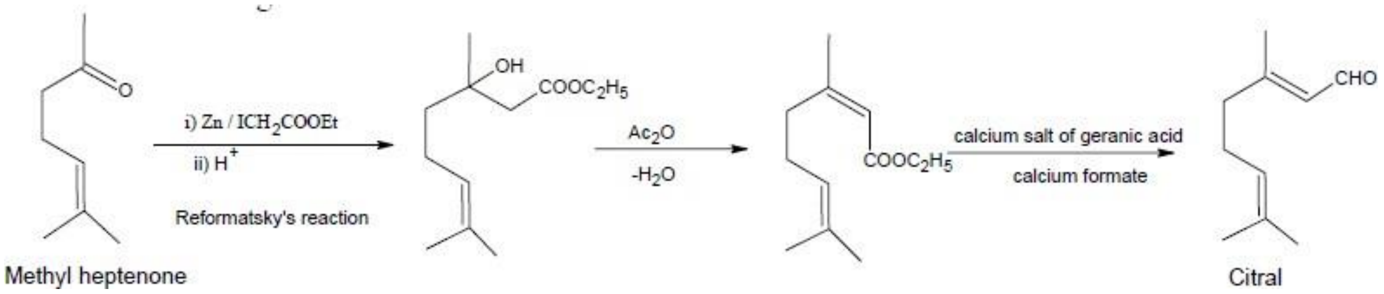
- **Citral** on boiling with **aqueous potassium carbonate** yielded **6-methyl hept-5-ene-2-one (Methylheptenone)** and **acetaldehyde**. The formation of these can only be explained on the basis of proposed structure;



It appears that citral is product of aldol condensation of these two.

SYNTHESIS OF CITRAL

***Barbier-Bouveault-Tiemann's synthesis*:** In this synthesis methyl heptenone is converted to geranic ester by using Reformatsky's reaction. Geranic ester is then converted to citral by distilling a mixture of calcium salts of geranic and formic acids.



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2. Organic Chemistry by Paula Yurkanis Bruice, 3rd edition.
3. Organic Chemistry by Robert T. Morrison and Robert Neilson Boyd, 6th edition.
4. Chemistry of Natural Products by S. V. Bhat, B. A. Nagasampagi and M. Siva Kumar

ALLOYS

Alloys and its applications

B.V.V.Sangha's
Basaveshwar Science College, Bagalkot
Department of Chemistry
B.Sc-V Semester

Paper Title: Chemistry-6
Paper Code : 21BSC5C5CHE6L

(e notes) by
Dr. (smt). S.R. Kaladagi
Associate professor

Unit –I
Industrial Chemistry –I

Alloys-Significance, types of alloys (ferrous and non-ferrous alloys), preparation (fusion and electro-deposition) and their applications.

INORGANIC CHEMISTRY

INDUSTRIAL CHEMISTRY

When a chemical reaction or series of chemical reactions are to be carried out any industry that uses large quantities of starting materials it is very much desirable that these reactions should be carried out under optimum conditions.

Industrial Chemistry is a branch of chemistry which deals with the preparation of chemical compounds as well as the extraction of metals from their ores.

a) ALLOYS

Most of the metals can be mixed up in all proportions, eg, tin and lead mix up in all proportion forming alloys. Alloys are formed not only by metals among themselves but also by metal and non metal. Thus**an alloy is a homogeneous mixture of two or more different elements, one of which at least is essentially a metal; hence it has metallic property.**

Alloys containing mercury (a liquid at ordinary temperature) as the constituent element, are called amalgams. eg: Sodium – amalgam is an alloy of sodium and mercury.

Generally alloys are harder, less malleable and have lower melting point than their component metals. They have low electrical conductivity and resist corrosion and the action of acids. Thus, the certain physical as well chemical properties of metals can be changed by alloying. A large number of metals have been used for making alloys and the important metals are Cu, Zn, Pb, Sn, Ni, Al, Cr, etc.

PURPOSE OF MAKING ALLOYS:

Pure metals in general possess a few useful physical properties like high malleability, ductility, lustre, good electrical conductivity etc. However, they are very soft and highly chemically reactive. The properties of a given metal can be improved by alloying it with some other metal or non-metal. The main purpose of making alloys are;

1) To enhance the hardness of the metal:

Pure metals are generally soft. The hardness of a metal is enhanced(increase) on alloying it with another metal or non-metal. In other words, an alloy is harder than its component elements. For example, addition of 0.5% arsenic makes lead so hard that it is used for making bullets.

2) To lower the melting point:

In general, the melting point of an alloy is lower that those of its constituent elements. For example, Wood's metal; it is an alloy of bismuth, lead, cadmium antin, possesses melting point of only 71°C which is much lesser than those of itscomponents Bi, Pd, Cd and Sn.

3) To enhance the tensile strength:

Alloy formation, in general, enhances the tensile strength of the parent or base metal (1.e. the major constituent of an alloy). For example, addition of the carbon increases the tensile strength of pure iron by about ten times.

iv) To enhance corrosion resistance:

Metals in pure form are quite reactive and easily corroded by surrounding atmospheric gases, moisture, etc. But alloys of such metals are more resistant to corrosion than pure metals. For example, iron is corroded even in moist air but stainless steel an alloy of Fe, Cr, C and Ni, is even acid-proof.

v) To modify color:

The color of metal can be modified to a desired one by alloying it with another suitable element. Thus, an alloy can be prepared having a colour quite different from the coloured of the base metals. For example, brass and alloy of copper (red) and zinc (silver white) is yellow in color.

vi) To modify chemical activity:

Chemical activity of metals may be increased or decreased by alloying. For example, sodium amalgam (NaHg) is less active than sodium while aluminum amalgam is more active than aluminum.

vii) To provide better castability:

One of the most essential requirements of getting good castings is expansion of metal on solidification. But pure molten metals in general undergo contraction on solidification. Hence, in order to get good castings, metals have to be alloyed, because alloys expand on solidification. For example, “Type metal” (an alloy of Pb, Sn and Sb), which is used for casting printing type. due to its exceptionally good casting properties.

TYPES OF ALLOYS:

Iron is one of the metals, referred to in the classification of alloys. Thus, alloys are classified into two types viz,

(a) Ferrous alloys
(b) Non-ferrous alloys

FERROUS ALLOYS (OR FERROALLOYS):

Ferro alloys are alloys of iron with metals like Mn, Cr, Ni, Mo W They are brittle and for unusual industrial applications. They are used mainly to introduce the alloying element into steel in the manufacture of alloy steels.

Main purpose of alloying steel are to improve tensile strength resistance, corrosion resistance, harden ability, weldability, shock resistance, , magnetic permeability, ability to retain physical properties at high temperature, and minimize the coefficient of expansion.

Important ferrous Alloys

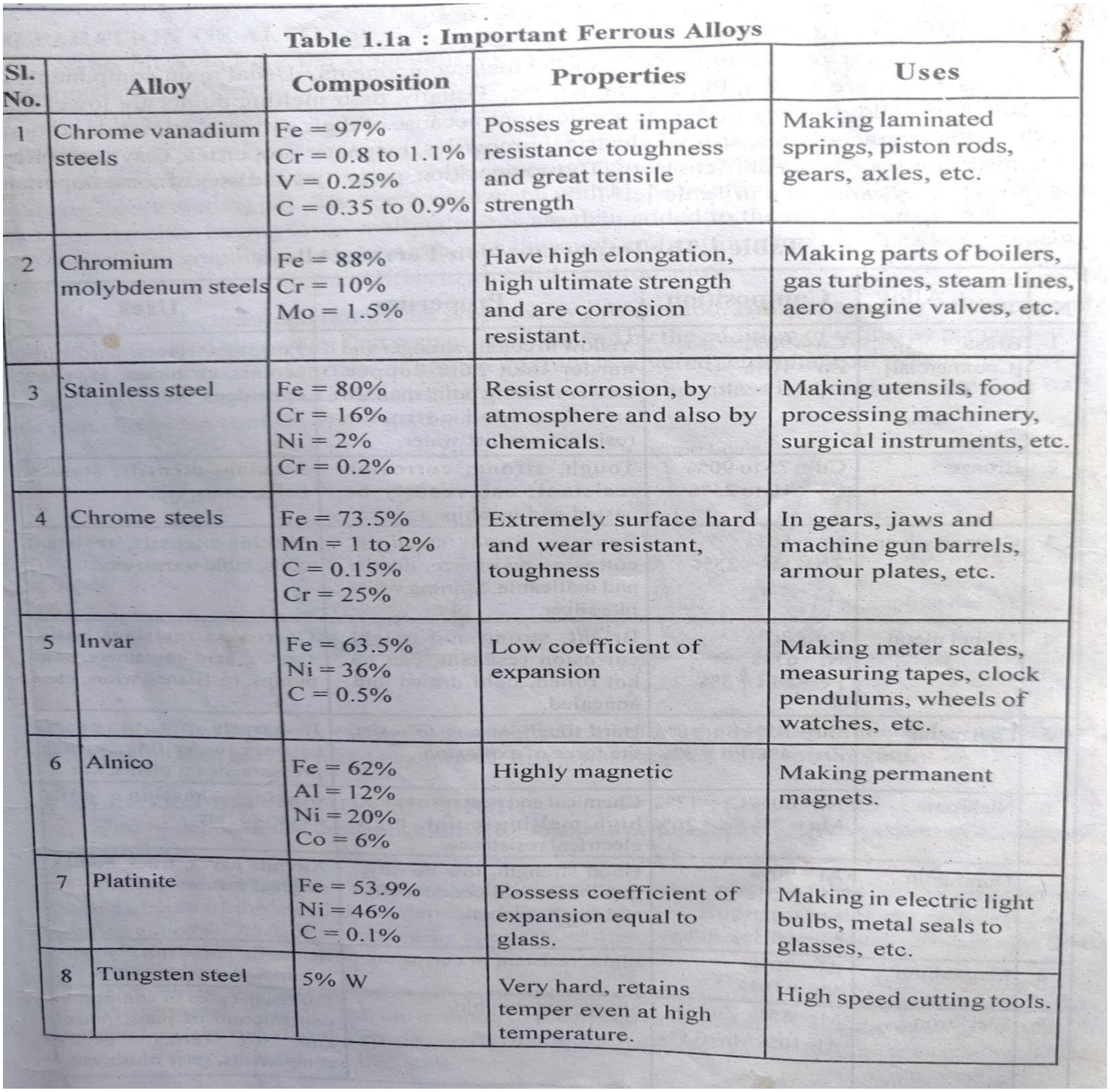
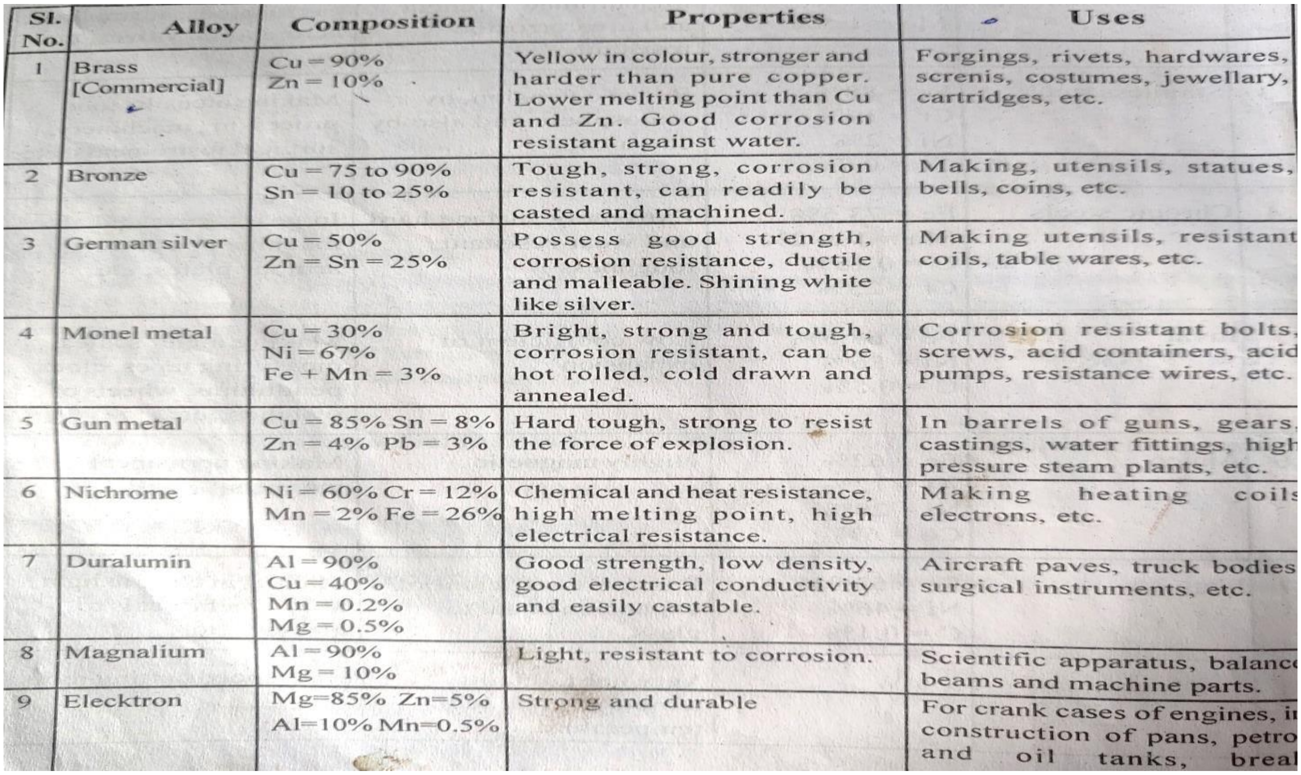


Table 1.1a : Important Ferrous Alloys

Sl. No.	Alloy	Composition	Properties	Uses
1	Chrome vanadium steels	Fe = 97% Cr = 0.8 to 1.1% V = 0.25% C = 0.35 to 0.9%	Posses great impact resistance toughness and great tensile strength	Making laminated springs, piston rods, gears, axles, etc.
2	Chromium molybdenum steels	Fe = 88% Cr = 10% Mo = 1.5%	Have high elongation, high ultimate strength and are corrosion resistant.	Making parts of boilers, gas turbines, steam lines, aero engine valves, etc.
3	Stainless steel	Fe = 80% Cr = 16% Ni = 2% Cr = 0.2%	Resist corrosion, by atmosphere and also by chemicals.	Making utensils, food processing machinery, surgical instruments, etc.
4	Chrome steels	Fe = 73.5% Mn = 1 to 2% C = 0.15% Cr = 25%	Extremely surface hard and wear resistant, toughness	In gears, jaws and machine gun barrels, armour plates, etc.
5	Invar	Fe = 63.5% Ni = 36% C = 0.5%	Low coefficient of expansion	Making meter scales, measuring tapes, clock pendulums, wheels of watches, etc.
6	Alnico	Fe = 62% Al = 12% Ni = 20% Co = 6%	Highly magnetic	Making permanent magnets.
7	Platinite	Fe = 53.9% Ni = 46% C = 0.1%	Possess coefficient of expansion equal to glass.	Making in electric light bulbs, metal seals to glasses, etc.
8	Tungsten steel	5% W	Very hard, retains temper even at high temperature.	High speed cutting tools.

NON-FERROUS ALLOYS:

These do not contain iron as one of the main components. Usual main components of non-ferrous alloys are Al, Cu, Pb, Zn, Sn, Ni, etc. Usually, their melting points are lower than those of ferrous alloys. They find wide applications because of their softness, attractive colours, cold-working characteristics, special electrical properties, magnetic properties, easy castability, low density, low coefficient of friction etc. The composition, properties and uses of some important non-ferrous alloys are given in Table



Sl. No.	Alloy	Composition	Properties	Uses
1	Brass [Commercial]	Cu = 90% Zn = 10%	Yellow in colour, stronger and harder than pure copper. Lower melting point than Cu and Zn. Good corrosion resistant against water.	Forgings, rivets, hardwares, screnis, costumes, jewellary, cartridges, etc.
2	Bronze	Cu = 75 to 90% Sn = 10 to 25%	Tough, strong, corrosion resistant, can readily be casted and machined.	Making, utensils, statues, bells, coins, etc.
3	German silver	Cu = 50% Zn = Sn = 25%	Possess good strength, corrosion resistance, ductile and malleable. Shining white like silver.	Making utensils, resistant coils, table wares, etc.
4	Monel metal	Cu = 30% Ni = 67% Fe + Mn = 3%	Bright, strong and tough, corrosion resistant, can be hot rolled, cold drawn and annealed.	Corrosion resistant bolts, screws, acid containers, acid pumps, resistance wires, etc.
5	Gun metal	Cu = 85% Sn = 8% Zn = 4% Pb = 3%	Hard tough, strong to resist the force of explosion.	In barrels of guns, gears, castings, water fittings, high pressure steam plants, etc.
6	Nichrome	Ni = 60% Cr = 12% Mn = 2% Fe = 26%	Chemical and heat resistance, high melting point, high electrical resistance.	Making heating coils electrons, etc.
7	Duralumin	Al = 90% Cu = 40% Mn = 0.2% Mg = 0.5%	Good strength, low density, good electrical conductivity and easily castable.	Aircraft paves, truck bodies surgical instruments, etc.
8	Magnalium	Al = 90% Mg = 10%	Light, resistant to corrosion.	Scientific apparatus, balanc beams and machine parts.
9	Elecktron	Mg=85% Zn=5% Al=10% Mn=0.5%	Strong and durable	For crank cases of engines, i construction of pans, petro and oil tanks, brea

PREPARATION OF ALLOYS:

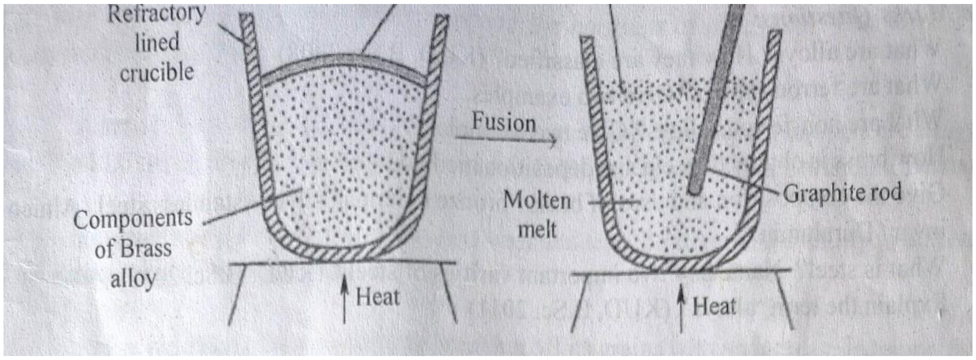
The following are the commonly employed methods for the manufacture of binary (two-component) alloys.

i) Fusion method ii) Electro deposition method

i) FUSION METHOD:

The components of the alloy in proper proportions are fused together in a fire clay refractory lined crucible or melting pot. The component metal with higher melting point is first melted and the other components, having lower melting points are then added to the melt. The molten mass is well stirred with graphite rods to bring about a thorough and uniform mixing. The homogeneous mass thus prepared on cooling solidifies to give the required alloy.

Alloys like brass and bronze are prepared by this method. Brass is an alloy of copper and zinc can be obtained by melting first copper and followed by the addition of requisite proportion of zinc in the solid form. The surface of molten mixture is covered with charcoal powder in order to avoid oxidation of copper and zinc in molten states. The molten mass is stirred with graphite rods and then allowed to cool slowly to get brass.



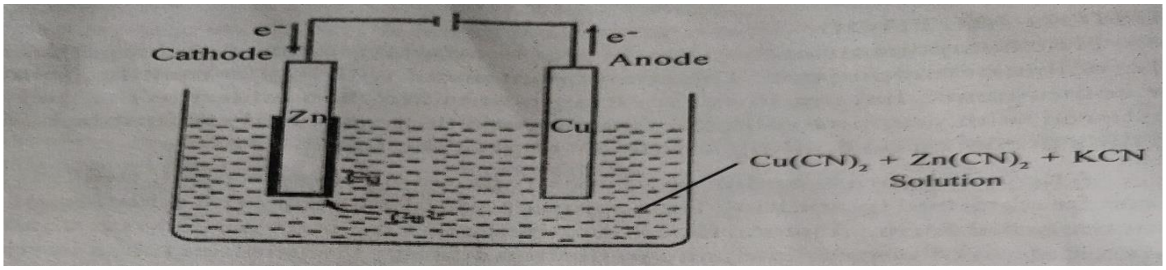
Note: If metal having lower melting point melts first before the melting of metal having higher melting point then the first metal evaporates, this is not happens in fusion method.

ii) ELECTRO-DEPOSITION METHOD:

Electro-deposition is the deposition of a substance on an electrode by the action of electricity by electrolysis.

During electrolysis, the metal on which deposition takes place is taken as cathode and the anode is made of the metal to be deposited on the cathode. Both electrodes are immersed in a solution called an electrolyte

containing one or more dissolved metal salts as well as other ions that permit the flow of electricity.
The anode and cathode are both connected to a battery. The anode is connected to the positive terminal of supply and the cathode to the negative terminal. When the external power is switched on, the metal at the anode is oxidized to form cations. These cations are reduced at the cathode to deposit in the metallic state.
Brass alloy can also be prepared by this method. A solution of copper all potassium cyanide is taken in an electrolytic cell and electric current is passed, so that proportion of copper and zinc get deposited on the cathode to give brass.



EXAMINATION QUESTIONS

Two Marks Questions: 1) What are alloys? How they are classified? (KUD, B.Sc. 2008)

2) What are ferrous alloys? Give two examples.

3) What are non-ferrous alloys

6) What is steel? Name any two important varities of steels. (KUD, B.Sc. 2011)

7) Explain the term “alloys'. (KUD, B.Sc. 2011)

Five Marks Question:

1) Discuss the purpose of making alloys. (KUD, B.Sc. 2010)

2) Discuss the applications of ferrous alloys. (KUD, B.Sc. 2009)

3) Discuss the applications of non-ferrous alloys. (KUD, B.Sc. 2010)

1) Give the composition and application of

(1) German silver (2) Commercial brass

2) How is brass manufactured by electrode deposition method? Give is composition and two applications? (KUD, B.Sc. 2008)

3) What are alloys? How are they classified? Give composition and applications of (1) Stainless steel (2) Brass (KUD, B.Sc. 2007)

Reference:

Industrial chemistry by B K Sharma.

B. V. V. Sangha's
BASAVESHWAR SCIENCE COLLEGE, BAGALKOT
DEPARTMENT OF PHYSICS

Semester: B.Sc. I Semester **Subject:** Physics
Unit-: MECHANICS AND PROPERTIES OF MATTER **Name: Mr. P. V. Koshti**

Course Code: 2A1PHYM01T

B.Sc I Semester

Paper-I MECHANICS AND PROPERTIES OF MATTER

Rigid body dynamics (13 hours)

Moment of inertia and its physical significance. Derivation for theorems of moment of inertia. Derivation of expression for moment of inertia of rectangular lamina, thin Uniform rod, Circular disc. Qualitative discussion on Moment of Inertia of Annular ring ,hollow and solid cylinders. Theory of bar pendulum and compound pendulum. Experimental determination of Moment of inertia of Fly wheel with relevant theory. Problems.

Inertia

Inertia is the resistance of any physical object to any change in its state of motion, including changes to its speed and direction. It is the tendency of objects to keep moving in a straight line at constant velocity. The principle of inertia is one of the fundamental principles of classical physics that are used to describe the motion of objects and how they are affected by applied forces. In common usage, the term "inertia" may refer to an object's "amount of resistance to change in velocity" (which is quantified by its mass), or sometimes to its momentum, depending on the context. The term "inertia" is more properly understood as shorthand for "the principle of inertia" as described by Newton in his First Law of Motion: that an object not subject to any net external force moves at a constant velocity. Thus, an object will continue moving at its current velocity until some force causes its speed or direction to change. On the surface of the Earth, inertia is often masked by the effects of friction and air resistance, both of which tend to decrease the speed of moving objects (commonly to the point of rest), and gravity. This misled classical theorists such as Aristotle, who believed that objects would move only as long as force was applied to them.

Classical inertia: The law of inertia states that it is the tendency of an object to resist a change in motion. According to Newton, an object will stay at rest or stay in motion (i.e. 'maintain its velocity' in modern terms) unless acted on by a net external force, whether it results from gravity, friction, contact, or some other source. The Aristotelian division of motion into mundane and celestial became increasingly problematic in the face of the conclusions of Nicolaus Copernicus in the 16th century, who argued that the earth (and everything on it) was in fact never "at rest", but was actually in constant motion around the sun. Galileo, in his further development of the Copernican model, recognized these problems with the then-accepted nature of motion and, at least partially as a result, included a restatement of Aristotle's description of motion in a void as a basic physical principle:

A body moving on a level surface will continue in the same direction at a constant speed unless disturbed.

Galileo writes that 'all external impediments removed, a heavy body on a spherical surface concentric with the earth will maintain itself in that state in which it has been; if placed in movement towards the west (for example), it will maintain itself in that movement'. This notion which is termed 'circular inertia' or 'horizontal circular inertia' by historians of science, is a precursor to, but distinct from, Newton's notion of rectilinear inertia. For Galileo, a motion is 'horizontal' if it does not carry the moving body towards or away from the centre of the earth, and for him 'a ship, for instance, having once received some impetus through the tranquil sea, would move continually around our globe without ever stopping'.

It is also worth noting that Galileo later went on to conclude that based on this initial premise of inertia, it is impossible to tell the difference between a moving object and a stationary one without some outside reference to compare it against.[19] This observation ultimately came to be the basis for Einstein to develop the theory of Special Relativity.

Mass and inertia

Physics and mathematics appear to be less inclined to use the popular concept of inertia as "a tendency to maintain momentum" and instead favor the mathematically useful definition of inertia as the measure of a body's resistance to changes in velocity or simply a body's inertial mass.

This was clear in the beginning of the 20th century, when the theory of relativity was not yet created. Mass, m, denoted something like an amount of substance or quantity of matter. And at the same time mass was the quantitative measure of inertia of a body.

The mass of a body determines the momentum p of the body at given velocity v; it is a proportionality factor in the formula:

$P = mv$ ---------(1)

The factor m is referred to as inertial mass.

But mass, as related to the 'inertia' of a body, can also be defined by the formula:

$F = ma$ ----------(2)

Here, F is force, m is inertial mass, and a is acceleration.By this formula, the greater its

mass, the less a body accelerates under given force. Masses defined by formula (1) and (2) are equal because formula (2) is a consequence of formula (1) if mass does not depend on time and velocity. Thus, "mass is the quantitative or numerical measure of a body’s inertia, that is of its resistance to being accelerated".

This meaning of a *body's inertia* therefore is altered from the popular meaning as "a tendency to maintain momentum" to a description of the measure of how difficult it is to change the velocity of a body. But it is consistent with the fact that motion in one reference frame can disappear in another, so it is the change in velocity that is important.

Rotational inertia

Another form of inertia is *rotational inertia* (→ moment of inertia), which refers to the fact that a rotating rigid body maintains its state of uniform rotational motion. Its angular momentum is unchanged, unless an external torque is applied; this is also called conservation of angular momentum. Rotational inertia depends on the object remaining structurally intact as a rigid body, and also has practical consequences; For example, a gyroscope uses the property that it resists any change in the axis of rotation.

Center of Mass

After developing kinematics of rotational motion, the rotational motion dynamics were developed. In this the parallel concepts are applied to linear dynamics which contains some unique concepts and equations. The main important concept in rotational dynamics is a torque. It also involves the study of work, power, and kinetic energy like in linear motion, moment of inertia, **centre of mass** and equations for a description of the combination of linear and angular motion.

Here we are discussing about the centre of mass. The terms centre of mass or gravity are used in a constant field of gravity which shows a specific point in the system. It is used to describe a response of the system towards the external force and torque. If we see in on dimension plane then it is similar to seesaw at a pivot point. It contains the total mass of the body at one point. Let’s discuss more about the centre of mass and the process of finding it.

Clock balancing on end of finger

This clock uses the principles of center of mass to keep balance on a finger.

Center of Mass - Defenition

A point where whole of the body’s mass can be assumed to be located or concentrated is called center of mass.

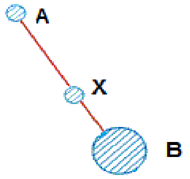
- The point can be real or imaginary, for example, in the case of a hollow or empty box the mass is physically not located at the center of mass point. This mass is supposed to be located at the center of mass in order to simplify calculations.
- The motion of the center of mass characterizes the motion of the entire object. The center of mass may or may not be the same to the geometric center if a rigid body is considered. It is considered as a reference point for many other

calculations of mechanics.The center of mass of a rigid body is a point whose position is fixed with respect to the body as a whole. The point may or may not lie in the body. The position of the center of mass of a rigid body depends on:

1. Shape of the body
2. Distribution of mass in the body

Center of Mass Equation

Consider two particles A and B of masses m_1 and m_2, respectively. Take the line joining A and B as the X-axis. Let the coordinates of the particles at time 't' be x_1 and x_2. Suppose no external force acts on the system. The particles A and B, however, exert forces on each other and these particles accelerate along the line joining them. Suppose the particles are initially at rest and the force between them is attractive.



The center of mass at time t is situated at $X = m_1x_1+m_2x_2/\ m_1+m_2$

Moment of inertia

For a point mass the **moment of inertia** is just the mass times the square of perpendicular distance to the rotation axis, $I = mr^2$. That point mass relationship becomes the basis for all other **moments of inertia** since any object can be built up from a collection of point masses.
OR

Moment of inertia is the name given to rotational inertia, the rotational analog of mass for linear motion. It appears in the relationships for the dynamics of rotational motion. The moment of inertia must be specified with respect to a chosen axis of rotation. For a point mass the moment of inertia is just the mass times the square of perpendicular distance to the rotation axis, $I = mr^2$. That point mass relationship becomes the basis for all other moments of inertia since any object can be built up from a collection of point masses.

OR Moment of Inertia

According to the first law of motion given by *Newton* says that a body is in its current motion state till any external force is acted upon it. The **moment of inertia** of the linear motion is measured by the mass of the system and angular counterpart. The inertia is related to mass and the amount of mass distribution throughout the body. It is not necessary to be possessing same moment of inertia by two bodies of the same mass. Thus, the inertia shows that how tough a body to move.

If an object possess more inertia then it is very to move it or stop it; for example, the inertia of heavy truck is more than a person. It also shows how hard is spinning of an object with respect to certain axis which depends on mass and location of mass. This spinning difficulty around an axis is the moment of inertia. Let’s discuss more on that.

Moment of Inertia- Definition

The concept of moment of inertia was introduced by *Leonhard Euler*. The resistance that is shown by the object to change its rotation is called **moment of inertia**. **I** and **J** are used as symbols for denoting moment of inertia.The moment of inertia describes the angular acceleration produced by an applied torque. It depends on the shape and mass distribution of the body, and on the orientation of the rotational axis.

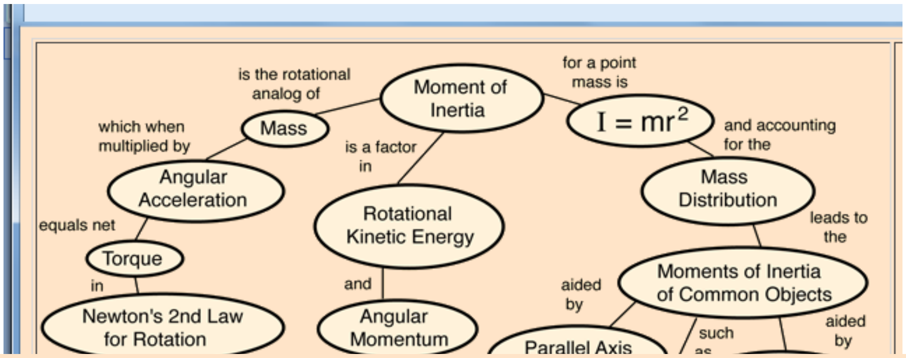
The moment of inertia plays the same role for rotation as the mass does for a translational motion, it describes the resistance of a body to a change of its state of motion. The difficulty faced to change the angular motion of any object about an axis is shown or given or measured by calculating moment of inertia about that particular axis.

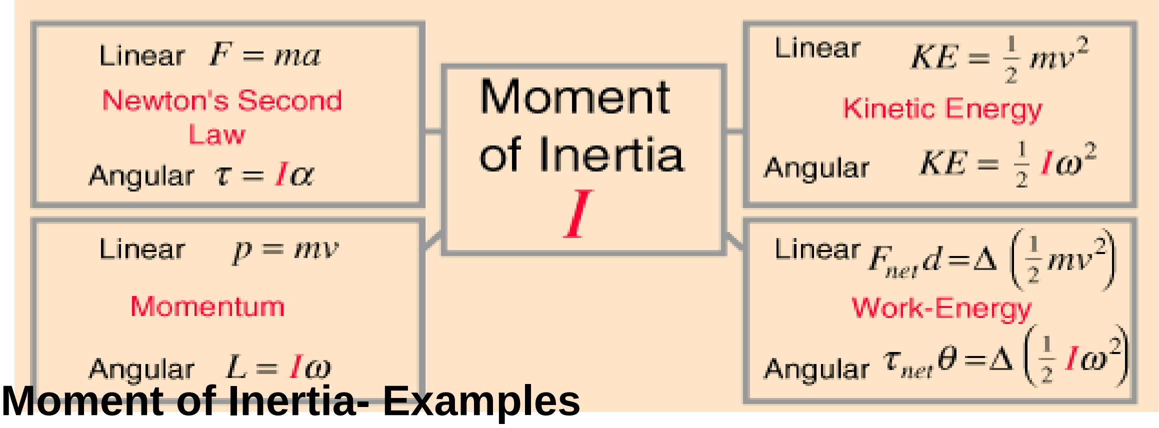
Moment of Inertia -Equation

Moment of inertia is given by the following equation,

$\mathbf{I = \sum m_i r_i^2}$ **............................**(a)

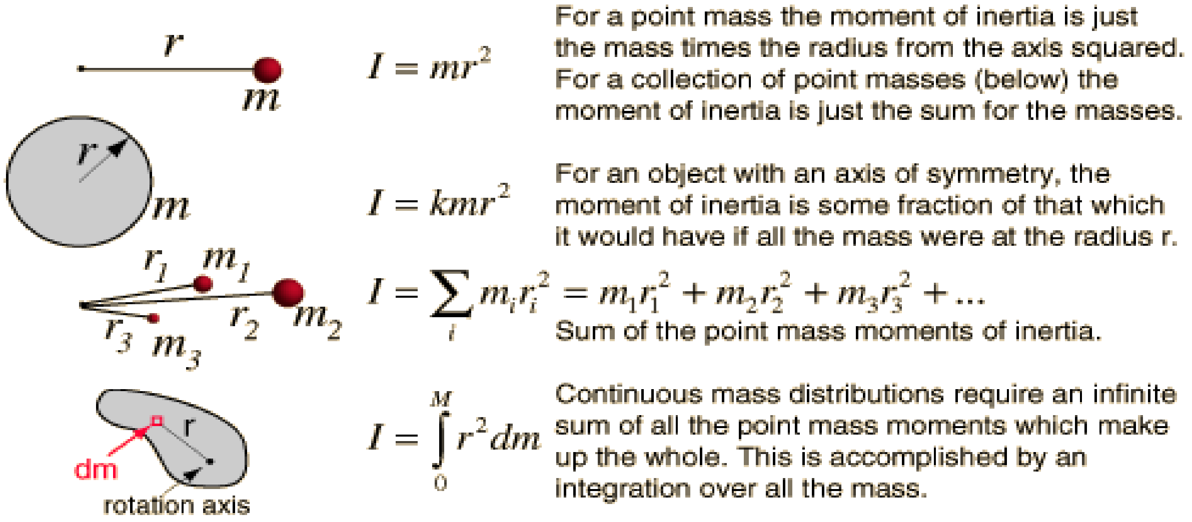
Here $\mathbf{r_i}$ is the distance to the axis on which rotation is done to any other point and not distance of the point to the origin.





Moment of Inertia- Examples

Moment of inertia is defined with respect to a specific rotation axis. The moment of inertia of a point mass with respect to an axis is defined as the product of the mass times the distance from the axis squared. The moment of inertia of any extended object is built up from that basic definition. The general form of the moment of inertia involves an integral.



$$I = mr^2$$

For a point mass the moment of inertia is just the mass times the radius from the axis squared. For a collection of point masses (below) the moment of inertia is just the sum for the masses.

$$I = kmr^2$$

For an object with an axis of symmetry, the moment of inertia is some fraction of that which it would have if all the mass were at the radius r.

$$I = \sum_i m_i r_i^2 = m_1 r_1^2 + m_2 r_2^2 + m_3 r_3^2 + \ldots$$

Sum of the point mass moments of inertia.

$$I = \int_0^M r^2\, dm$$

Continuous mass distributions require an infinite sum of all the point mass moments which make up the whole. This is accomplished by an integration over all the mass.

Radius of gyration

- Whatever may be the shape of the body it is always possible to find a distance from the axis of rotation at which whole mass of the body can be assumed to be concentrated and even then its moment of inertia about that axis remains unchanged.
- If whole mass of the body is supposed to be concentrated at a distance k from the axis of rotation then
  $I=Mk^2=\Sigma mr^2$
  or ,
  $k=\sqrt{(I/M)}=\sqrt{(\Sigma mr^2/M)}$
  This quantity k is called radius of gyration of the body about the axis of rotation.
- Thus, the radius of gyration of a body, rotating about a given axis of rotation is the radial distance from the axis and when the square of radius of gyration (k) is multiplied by the total mass of the body it gives the moment of inertia of the body about that axis.

Torque

Torque is a turn or twist force acting. Lets have a simply illustration to know that. When we apply the force the door turns on its hinges. Thus a turning effect is produced when we try to open the door. Have you ever tried to do so by applying the force near the hinge?
In the first case, we are able to open the door with ease. In the second case, we have to apply much more force to cause the same turning effect. What is the reason?
This turning effect produced by a force on a rigid body about a point, pivot or fulcrum is called the moment of a force or **Torque**.

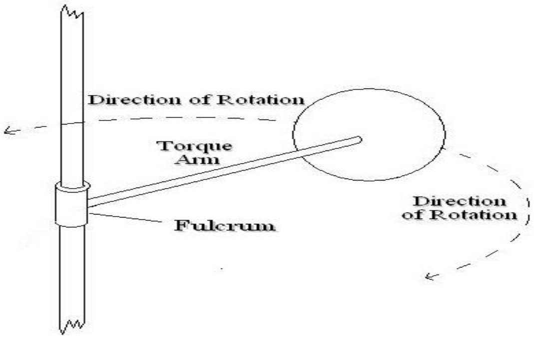
What is Torque ?

The Rate at which there is a change in angular momentum is also called **Torque**. It can also be defined as a twist to an object.

When we multiply the magnitude of force or the force's magnitude and the perpendicular distance of the line of action of the force from the axis of rotation then we get a quantity which is called **Torque.**

> “*The Rate at which there is a change in angular momentum is also called* ***Torque****. It can also be defined as a twist to an object.”*

When we multiply the magnitude of force or the force's magnitude and the perpendicular distance of the line of action of the force from the axis of rotation then we get a quantity which is called **Torque.**



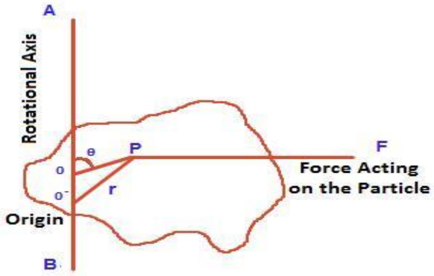
Mathematically, it can be defined as:
Torque = Perpendicular distance from the axis of rotation x Force.
τ = r x F.
= r F sinθ.
where,
r = a distance between the point from which torque is measured to the point where force is applied.
τ is the torque and
F = force applied
Its dimensional formula is **[M L^2 T^{-2}]**, which is same as that of work.

Torque Symbol :

Torque is denoted by the symbol τ. It is a Greek letter. It is pronounced as **‘tau’**.

Torque Equation

Consider a rigid body which is rotating about a given axis of rotation on which force is applied. Let us choose an origin **"O"** and let **"r"** be the position vector of the particle on which the force is applied.
Consideration a rigid body, which is rotating about a given axis of rotation **AB** as shown in figure.



where
AB is rotational axis,
O is the origin,
O and **O'** are the two points on the rotational axis,
θ is the angle between plane **AOB** and force **F**

Let **F** be the force acting on the particle **O** of the object or the body. **F** need not necessarily be in the plane **ABP**. Considering origin **O** approximately on the axis of rotation.

The torque of **F** about **O** is, $\tau = r \times F$ Its component along **OA** is called the torque of about **OA**.

To calculate it, we should find the vector $r \times F$ and then find out the angle θ it makes with **OA**. The torque about **OA** is then $|r \times F|$, the torque of a force about a line. This can be shown as given below. Let **O** be any point on the line **AB** (Figure b).

The torque of **F** about **O'** is,

$O'P \times F = (O'O + OP) \times F$

$= O'O \times F + OP \times F$ ....(a)

As this term will have no component along AB. Thus, the component of $O'P \times F$ is equal to that of $O'P \times F$

Also, $\tau = dL/dt$

which is the rate of change of angular momentum. This torque mentioned here is basically the net torque, i.e.,

$\tau 1 + \tau 2 + \tau 3 + \tau 4$ + so on $= dL/dt$

Hence,

$\tau net = dL/dt = d(I\alpha)/dt$

$= I\, d\alpha/dt$

$= I\,\alpha$

$\tau = I\,\alpha$ ....(c)

Where,
I is the moment of inertia and
α is the angular acceleration
This is called **Torque Formula**

Moment of Inertia and its significance

According to newton's first law of motion the body continues to stay in the state of rest or in the state of motion. This property of inertia possessed by all the matter is the measures of mass in translatory motion. Similarly when a body is rotating or fixed about an axis. Any change in its state of rest or motion can be brought about by a couple or Torque the greater the opposition to change greater is the inertia. It is this rotational inertia of the body is called its moment of inertia aboutits axis of rotation.

The analogy between the two types of motion is the mass defined as " Coefficient of inertia for translatory motion" and the moment of inertia defined as "Coefficient of rotational inertia in rotating motion". In translatory motion the motion of the body depends on the mass alone.

In rotatory motion, the moment of inertia of the body depends not only on the mass of the body but also upon the effective distance of the body from the axis of rotation. The effective distance K of the particles from the axis of rotation is called the radius of gyration about that axis and is equal to root mean square distance of the particles from the axis.

"The radius of gyration of a body about a given axis of rotation is the distance from the axis of rotation is the distance from the axis at which if the whole mass of the body were to be concentrated, the moment of inertia of the body about the axis of rotation would be the same as with the actual distribution of mass.

The mass of body remains the same, irrespective of rotation, the value of radius of gyration about the axis dependsupon.

a) The position and direction of the axis of rotation
b) The distribution of the mass of the body about this axis, the value for the same body is different at different inclination.

The radius of gyration of a body about a given axis of rotation given an inclination of the distribution of the mass of the body about it and hence the effect of distribution mass on the moment of inertia about that axis.

OR

Physical significance of moment of inertia

In linear motion, force acting on a body is, Force = mass x linear acceleration
= ma
The rotational motion, torque acting on the body is, Torque = moment of inertia x
angular acceleration=I□

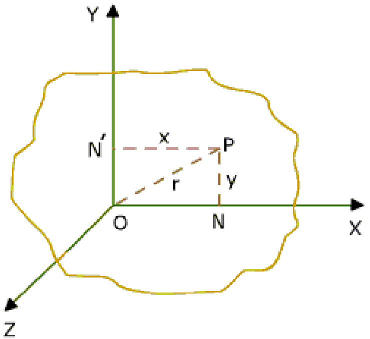
To set the body into linear motion, a force must be applied on it. In a similar way, to set a body into rotational motion, a torque must be applied on it.Thus torque is a quantity in rotational motion, analogous to the force intranslational, motion. Linear acceleration is the rate of change of linear velocity andangular acceleration is the rate of change of angular velocity. Therefore, linear ,acceleration and angular acceleration are analogous.

Comparing equation shows that the *I* moment of inertia is a quantity in rotational motion analogous to mass in translational motion. In linear motion, mass represent inertia of body. i.e. the tendency to maintain state of rest or of uniform motion, or to oppose the change in its state of rotational motion.

The moment of inertia in rotational motion, plays same role as inertial in linear motion. The tendency of a body to oppose any change in its state of rotation. It is also, known as rotational inertia: This is the physical significance of moment of inertia.

Perpendicular Axis Theorem

This is applicable only to a plane lamina. The moment of inertia of a plane lamina about an axis perpendicular to its plane is equal to the sum of the moments of inertia of the lamina about any two mutually perpendicular axes, passing in its own plane, intersecting each other at the point through which the perpendicular axis passes.



Theorem of perpendicular axis

Let us consider a plane lamina lying in the XOY plane. The lamina is made up of a large number of particles. Consider a particle of mass 'm' at P. From P, PN and PN^l are drawn perpendicular to X-axis and Y-axis, respectively.

Now $PN^l = x$, $PN = y$

Moment of inertia about X-axis = my^2

Moment of inertia of the whole of lamina about X-axis

$$I_x = \Sigma my^2$$

Moment of inertia of the whole of lamina about Y-axis

$$I_y = \Sigma mx^2$$

Moment of inertia of the whole of lamina about Z-axis

$$I_z = \Sigma mr^2$$

$$\text{But } r^2 = x^2 + y^2$$

$$\therefore I_z = \Sigma m\left(x^2 + y^2\right)$$

$$= \Sigma mx^2 + \Sigma my^2 \quad \text{or} \quad I_z = I_y + I_x$$

Parallel axes theorem

The moment of inertia I of a body about any axis is equal to the moment of inertia I_G about a parallel axis through the centre of gravity of the body plus Mb^2, where M is the mass of the body and b is the distance between the two axes. (See Figure 1**)**

$$I = I_G + Mb^2$$

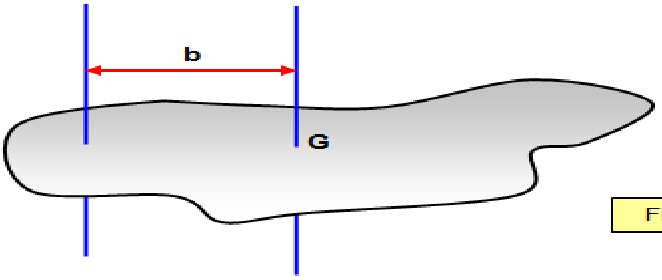
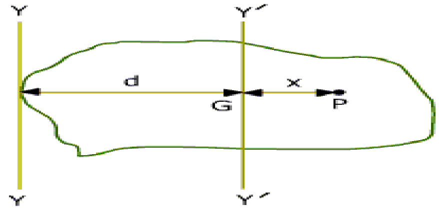


Figure 1

Parallel Axis Theorem

The moment of inertia of a body about an axis is equal to its moment of inertia about a parallel axis through its centre of gravity plus the product of the mass of the body and the square of the perpendicular distance between the two parallel axes.



Theorem of parallel axes

Let 'I' be the moment of inertia of a plane lamina about an axis YY. Let 'G' be the centre of gravity of the lamina. Y^{I} Y^{I} is an axis parallel to YY and passing through 'G'. Let 'I_g' be the moment of inertia of the lamina about Y^{I} Y^{I}.

Let GP = x.

Moment of inertia of the particle about

$Y\ Y = m\,(x + d)^2$

Moment of inertia of the whole of lamina about

$$YY = I = \sum m\,(x + d)^2$$

$$= \sum m\left(x^2 + d^2 + 2xd\right)$$

$$\Rightarrow I = \sum m\,x^2 + \sum md^2 + \sum 2mxd$$

But $\Sigma m x^2 = I_g$, $\Sigma md^2 = (\Sigma m)\, d^2 = Md^2$

Also $\Sigma 2mxd = 2d\Sigma mx$ $\therefore I = I_g + md^2 + 2d\Sigma mx$

The lamina will balance itself about its centre of gravity. So the algebraic sum of the moments of the **weights of constituent particles** about the centre of gravity G should be zero.

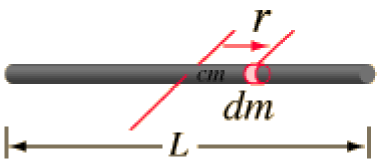
$\therefore \Sigma mg \times x = 0$ or $g\Sigma mx = 0$

$\Rightarrow \Sigma mx = 0$

$\therefore I = I_g + Md^2$

Moment of Inertia: Rod

Calculating the moment of inertia of a rod about its center of mass is a good example of the need for calculus to deal with the properties of continuous mass distributions. The moment of inertia of a point mass is given by I = mr^2, but the rod would have to be considered to be an infinite number of point masses, and each must be multiplied by the square of its distance from the axis. The resulting infinite sum is called an integral. The general form for the moment of inertia is:



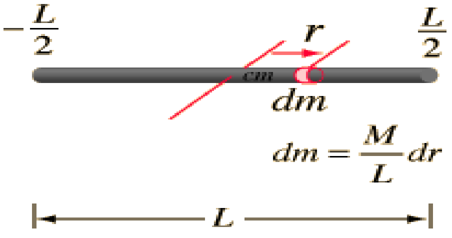
$$I = \int_0^M r^2\,dm$$

When the mass element dm is expressed in terms of a length element dr along the rod and the sum taken over the entire length, the integral takes the form:

$$I = \int_{-L/2}^{L/2} r^2 \frac{M}{L}\,dr = \frac{1}{12} ML^2$$

Rod Moment Calculation

The moment of inertia calculation for a uniform rod involves expressing any mass element in terms of a distance element dr along the rod. To perform the integral, it is necessary to express eveything in the integral in terms of one variable, in this case the length variable r. Since the total length L has mass M, then M/L is the proportion of mass to length and the mass element can be expressed as shown. Integrating from -L/2 to +L/2 from the center includes the entire rod. The integral is of polynomial type:



Total mass of rod: M

Linear density of rod: $\frac{M}{L}$

$$I = \int_{-L/2}^{L/2} r^2 \frac{M}{L} dr = \frac{M}{L}\frac{r^3}{3}\bigg|_{-L/2}^{L/2} = \frac{M}{3L}\left[\frac{L^3}{8} - \frac{-L^3}{8}\right]$$

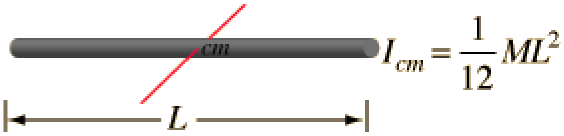
Mass of intinitesmal length dr :

$$dm = \frac{M}{L}dr$$

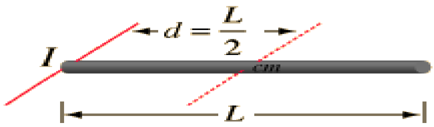
$$I_{cm} = \frac{1}{12}ML^2$$

Rod Moment About End

Once the moment of inertia of an object about its center of mass has been determined, the moment about any other axis can be determined by the Parallel axis theorem:



$$I = I_{cm} + Md^2$$

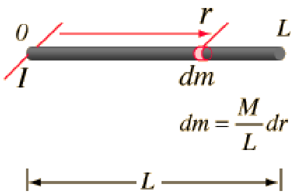


In this case that becomes

$$I_{end} = \frac{1}{12}ML^2 + M\frac{L^2}{4} = \frac{1}{3}ML^2$$

This can be confirmed by direct integration

$$I = \int_0^L r^2 \frac{M}{L} dr = \frac{M}{L}\frac{r^3}{3}\bigg|_0^L = \frac{1}{3}ML^2$$



Moment of inertia of the uniform circular plate about its axis

- Consider a uniform circular plate of mass M and radius R as shown below in the figure

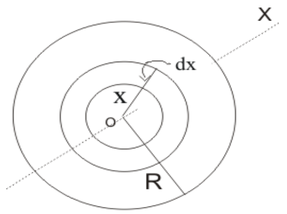


Figure 5. Uniform circular plate of mass M and radius R

- Let O be the center of the plate and OX is the axis perpendicular to the plane of the paper
- To find the moment of inertia of the plate about the axis OX draw two concentric circles of radii x and x+dx having these centers at O,so that they form a ring
- Area of this ring is equal to its circumference multiplied by its width i.e.
  Area of the ring =2πxdx
- Mass of the ring would be

$$= \frac{M}{\pi R^2} 2\pi x dx = \frac{2Mxdx}{R^2}$$

- Moment of inertia of this ring about axis OX would be

$$\text{MI of the ring } = \frac{2Mxdx}{R^2} x^2 = \frac{2Mx^3 dx}{R^2}$$

- Since whole disc can be supposed to be made up of such like concentric rings of radii ranging from O to R ,we can find moment of inertia I of the disc by integrating moment of inertia of the ring for the limits x=0 and x=R

$$\therefore MI = \int_0^R \frac{2M}{R^2} x^3 dx$$

$$= \frac{2M}{R^2} \left[\frac{x^4}{4} \right]_0^R = \frac{2M}{R^2} \frac{R^4}{4} = \frac{MR^2}{2}$$

Reference:

1. Fundamentals of Physics – R.Resnik, D. Halliday and Walikar; Wiley (2001).
2. Properties of Matter- J C Upadhya, Himalaya (2014ed).
3. Mechanics – Berkeley Physics Course
4. Physics- Classical and Modern, FJ Keller, E Gettys and J J Skove.
5. Concepts of Physics Vl(1)- H C Verma, Bharathi Bhavan Publishers, 2004.

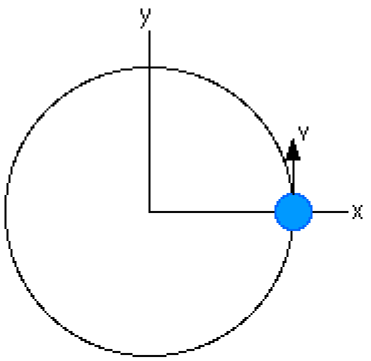
B. V. V. Sangha's
BASAVESHWAR SCIENCE COLLEGE, BAGALKOT
DEPARTMENT OF PHYSICS

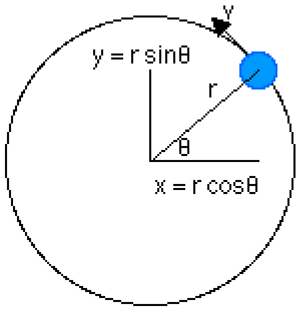
Semester: B.Sc. I Semester **Subject:** Physics

Unit: SIMPLE HARMONIC MOTION **Name:** Prof. (Smt.) V. N. Vanakudure

Course Code: 2A1PHYM01T

SIMPLE HARMONIC MOTION (13 hours)





The motion is uniform circular motion, meaning that the angular velocity is constant, and the angular displacement is related to the angular velocity by the equation:

$$\theta = \omega t$$

Plugging this in to the x and y positions makes it clear that these are the equations giving the coordinates of the object at any point in time, assuming the object was at the position x = r on the x-axis at time = 0:

$$x = r \cos\omega t \qquad \text{and } y = r \sin\omega t$$

How does this relate to simple harmonic motion? An object experiencing simple harmonic motion is traveling in one dimension, and its one-dimensional motion is given by an equation of the form

$$x = A \cos\omega t, \qquad \text{where A is the amplitude of the motion.}$$

The amplitude is simply the maximum displacement of the object from the equilibrium position.

So, in other words, the same equation applies to the position of an object experiencing simple harmonic motion and one dimension of the position of an object experiencing uniform circular motion. Note that the ω in the SHM displacement equation is known as the angular frequency. It is related to the frequency (f) of the motion, and inversely related to the period (T):

$$\text{For SHM}: \quad \omega = 2\pi f = 2\pi / T \qquad (\text{so } f = 1 / T)$$

The frequency is how many oscillations there are per second, having units of hertz (Hz); the period is how long it takes to make one oscillation.

Velocity in SHM

In simple harmonic motion, the velocity constantly changes, oscillating just as the displacement does. When the displacement is maximum, however, the velocity is zero; when the displacement is zero, the velocity is maximum. It turns out that the velocity is given by:

$$v = -A\omega \sin\omega t, \qquad \text{so the maximum speed is } A\omega$$

Acceleration in SHM

The acceleration also oscillates in simple harmonic motion. If you consider a mass on a spring, when the displacement is zero the acceleration is also zero, because the spring applies no force. When the displacement is maximum, the acceleration is maximum, because the spring applies maximum force; the force applied by the spring is in the opposite direction as the displacement. The acceleration is given by:

$$a = -A\omega^2 \cos\omega t, \qquad \text{so the maximum acceleration is } A\omega^2$$

Differential Equation of Equation of SHM

- Consider any particle executing SHM with origin as it's equilibrium position under the influence of restoring force F=
- kx, where k is the force constant and x is the displacement of particle from the equilibrium position.
- Now since F= -kx is the restoring force and from Newton's law of motion force is give as F=ma, where m is the mass of the particle moving with acceleration a. Thus acceleration of the particle is

  $$a = F/m$$
  $$= -kx/m$$

  but we know that acceleration $a = dv/dt = d^2x/dt^2$

  $$\Rightarrow \quad d^2x/dt^2 = -kx/m \qquad (1)$$

  This equation 1 is the equation of motion of SHM.
- If we choose a constant $\varphi=\sqrt{(k/m)}$ then equation 1 would become

  $$d^2x/dt^2 = -\varphi^2 x \qquad (2)$$

- This equation is a differential equation which says that displacement x must be a funcyion of time such that when it's second derivative is calculated the result must be negative constant multiplied by the original function.
- Sine and cosine functions are the functions satisfying above requirement and are listed as follows

$$x = A \sin\omega t \qquad (3a)$$

$$x = A \cos\omega t \qquad (3b)$$

$$x = A \cos(\omega t+\varphi) \qquad (3c)$$

  each one of equation 3a, 3b and 3c can be submitted on the left hand side of equation 2 and can then be solved for verification.
- Conveniently we choose equation 3c i.e., cosine form for representing displacement of particle at any time t from equilibrium position. Thus,

$$x = A \cos(\omega t+\varphi) \qquad (4)$$

  and A , φ and φ are all constants.
- Fig below shows the displacement vs. time graph for phase $\varphi=0$.

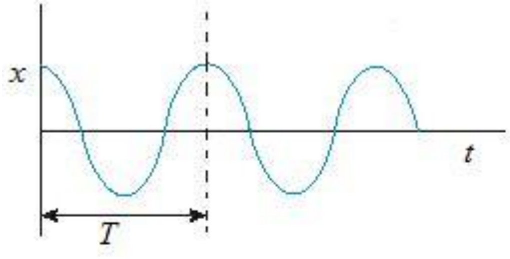


Figure 1

4. Characteristics of SHM

Here in this section we will learn about physical meaning of quantities like A, T, ω and φ.

(a) Amplitude

- Quantity A is known as amplitude of motion. it is a positive quantity and it's value depends on how oscillations were started.
- Amplitude is the magnitude of maximum value of displacement on either side from the equilibrium position.
- Since maximum and minimum values of any sine and cosine function are +1 and -1 , the maximum and minimum values of x in equation 4 are +A and -A respectively.
- Finally A is called the amplitude of SHM.

(b) Time period

- Time interval during which the oscillation repeats itself is known as time period of oscillations and is denoted by T.
- Since a particle in SHM repeats it's motion in a regular interval T known as time period of oscillation so displacement x of particle should have same value at time t and t+T. Thus,

$$\cos(\omega t+\varphi)=\cos(\omega(t+T)+\varphi)$$

  cosine function $\cos(\omega t+\varphi)$ will repeat it's value if angle $(\omega t+\varphi)$ is increased by 2π or any of its multiple. As T is the pime period

$$(\omega(t+T)+\varphi)=(\omega t+\varphi)+2\pi$$

  Or, $T=2\pi/` = 2\pi\sqrt{(m/k)}$ (5)
- Equation 5 gives the time period of oscillations.
- Now the frequency of SHM is defined as the number of complete oscillations per unit time i.e., frequency is reciprocal of time period.

$$f=1/T = 1/2\pi(\sqrt{(k/m)}) \qquad (6)$$

Thus, ω=2`/T = 2`f (7)

- This quantity ω is called the angular frequency of SHM.
- S.I. unit of T is s (seconds)
  f is Hz (hertz)
  ω is rad s^{-1} (radian per second)

(c) Phase

- Quantity (ωt+φ) in equation (4) is known as phase of the motion and the constant φ is known as initial phase i.e., phase at time t=0, or phase constant.
- Value of phase constant depends on displacement and velocity of particle at time t=0.
- The knowledge of phase constant enables us to know how far the particle is from equilibrium at time t=0. For example,
  If φ=0 then from equation 4

  $$x = A \cos\omega t$$

  that is displacement of oscillating particleis maximum , equal to A at t=0 when the motion was started. Again if φ=`/2 then from equation 4

  x = A cos(ωt+`/2)

  $$=A\sin\omega t$$

  Which means that displacement is zero at t = 0.

- Variation of displacement of particle executing SHM is shown below in the fig.

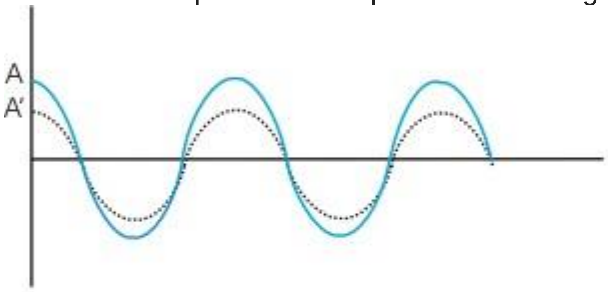


Figure 1a:- Figure shows the displacement Vs time graph for different amplitudes where A>A'

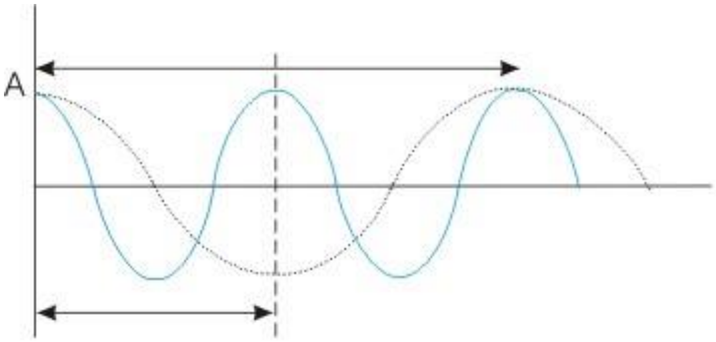


Figure 1b:- Figure shows the graph of SHM with different time periods where T′=T/2

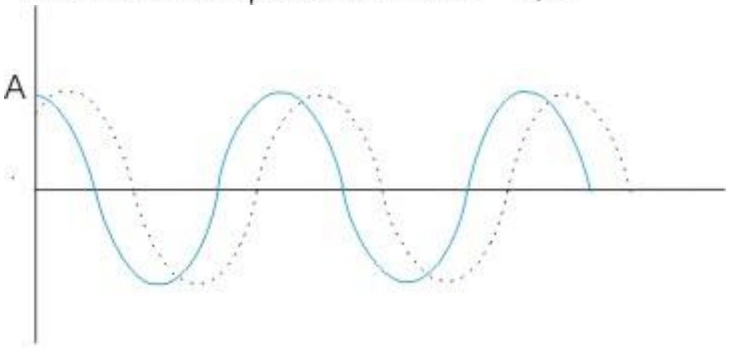


Figure 1c:- Figure shows SHM with different initial phase φ

5. Velocity of SHM

- We know that velocity of a particle is given by
  $v=dx/dt$
- In SHM displacement of particle is given by
  $x=A\cos(\omega t+\varphi)$
  now differentiating it with respect to t
  $v=dx/dt= A\omega(-\sin(\omega t+\varphi))$ (8)
- Here in equation 8 quantity Aω is known as velocity amplitude and velocity of oscillating particle varies between the limits ±ω.
- From trignometry we know that
  $\cos^2\theta + \sin^2\theta=1$
  ⇒
  $A^2 \sin^2(\omega t+\varphi)= A^2- A^2\cos^2(\omega t+\varphi)$
  Or
  $\sin(\omega t+\varphi)=[1-x^2/A^2]$ (9)
  putting this in equation 8 we get,

  $$v=-\omega A\left(1-\frac{x^2}{A^2}\right)^{1/2}$$

- From this equation 10 we notice that when the displacement is maximum i.e. ±A the velocity v=0, because now the oscillator has to return to change it� direction.

- Figure below shows the variation of velocity with time in SHM with initial phase φ=0.

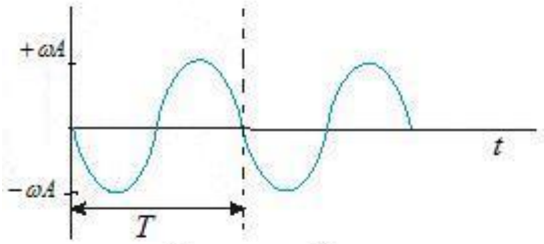


Figure 3

6. Acceleration of SHM

- Again we know that acceleration of a particle is given by
  a=dv/dt
  where v is the velocity of particle executing motion.
- In SHM velocity of particle is give by,
  v= -ωsin(ωt+φ)
  differentiating this we get,

  $$a = \frac{d}{dt}(-\omega A \sin(\omega t + \varphi))$$

  or,
  $a=-\omega^2 A\cos(\omega t+\varphi)$ (11)
- Equation 11 gives acceleration of particle executing simple harmonic motion and quantity ω^2 is called acceleration amplitude and the acceleration of oscillating particle varies betwen the limits $\pm\omega^2 A$.
- Putting equation 4 in 11 we get
  $a=-\omega^2 x$ (12)
  which shows that acceleration is proportional to the displacement but in opposite direction.
- Thus from above equation we can see that when x is maximum (+A or -A), the acceleration is also maximum($-\omega^2 A$ or $+\omega^2 A$)but is directed in direction opposite to that of displacement.

Figure below shows the variation of acceleration of particle in SHM with time having initial phase φ=0.

Reference:

1. Fundamentals of Physics – R.Resnik, D. Halliday and Walikar; Wiley (2001).
2. Properties of Matter- J C Upadhya, Himalaya (2014ed).
3. Mechanics – Berkeley Physics Course
4. Physics- Classical and Modern, FJ Keller, E Gettys and J J Skove.
5. Concepts of Physics Vl(1)- H C Verma, Bharathi Bhavan Publishers, 2004.

B. V. V. Sangha's

BASAVESHWAR SCIENCE COLLEGE, BAGALKOT

DEPARTMENT OF PHYSICS

Semester: B.Sc. I Semester **Subject:** Physics

Unit-: Surface Tension **Name:** Smt. L.S. Ganjal

Course Code: 2A1PHYM01T

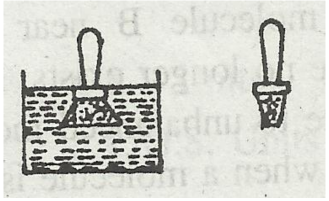
………

Surface tension (13Hours)

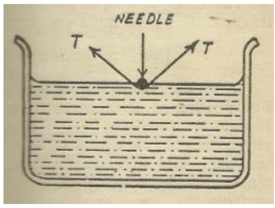
A stretched body is in a state of tension and has a natural tendency to contract. For example when we stretch a rubber tube it has a tendency to reduce its area. On account of the cohesive forces between the molecules of a liquid the free surface of a liquid always behaves like a stretched membrane or sheet and tends to contract to the smallest possible area. Since for a given volume a sphere has the least surface area, the liquid assumes a spherical shape. This is why the rain drop and mercury globules are spherical, that means we can say that every line in the free surface of a liquid is under tension. This is known as surface tension.

Observations illustrating surface tension

1. If a point brush dipped in water its hairs will be seen separately spread out. As we take it out the hairs come closer together because of the contracting tendency of the water film between the adjacent hairs.

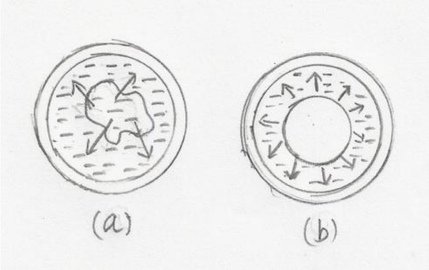


2. If we place a greased needle on a piece of blotting paper and put the paper lightly on the surface of the water the blotting paper will soon sink to the bottom, but the needle is found to float on the surface although it is much heavier than water. This is because the needle which is slightly depressed as if the liquid surface where acting as a stretched membrane, so that the weight of the needle is balanced by the inclined upward tension forces in the membrane.



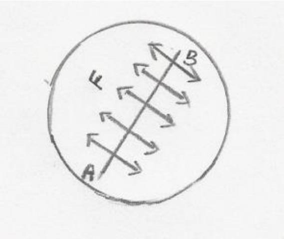
3. A circular ring of a thin wire is immersed in a soap solution and then taken out. A very thin soap film is seen to be formed within the ring. A loop of thread is gently kept on the film

without disturbing the film. The loop floats shapelessly on the film (fig a). When the film inside the loop is broken the film surrounding the loop, due to its tendency to shrink pulls the tread and the loop takes a circular shape (fig b). This indicates that the pull is equal in all direction.



Surface tension (Definition and Expression)

We have seen that a liquid has a tendency to minimize its surface area and hence any line in the surface of the liquid is under tension.



Let us imagine a straight line AB of length ‘ l ’drawn in the free surface of a liquid, then on account of tension of the liquid surface, the molecules on the two sides of the line will be a tendency o pull away from each other. The direction of the pulling force is at right angle to AB and tangential tote liquid surface. The magnitude of this force is found to be proportional to the length of the line. Thus if ‘F’ be the force acting at right angles on either side of the line AB.

Then $F \alpha l$ $F = Tl$ Or $T = \frac{F}{l}$

Where T is a constant for a liquid at a particular temperature. This constant is called tension of the liquid.

If l=1 unit F=T

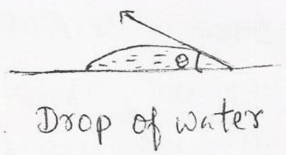
Thus “surface tension of a liquid is defined as the tangential force per unit length, acting at right angle on either side of a line imagined to be drawn in the free liquid surface in equilibrium”

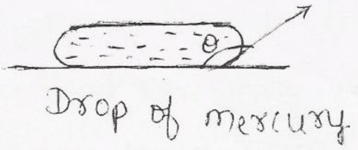
The unit of surface tension is dynes cm^{-1} in C.G.S system and $N - m^{-1}$ in S.I system. The dimension of surface tension is $\left[M^{1} L^{o} T^{-2}\right]$

Angle of contact

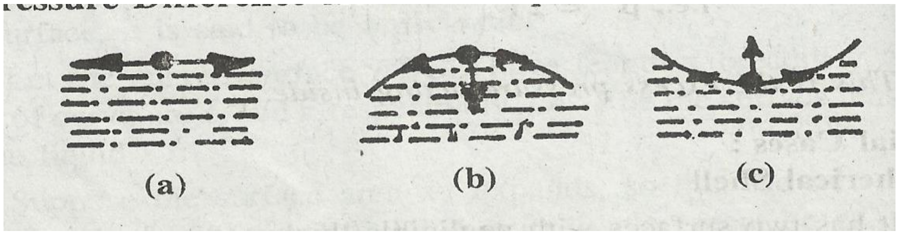
When a liquid is in contact with a solid, the surface of the liquid will be curved at the point of contact. “The angle of contact is defined as the angle between the tangent to the liquid surface drawn at the point of contact and the solid surface inside the liquid”.

Angle of contact is usually considered for a pair of solid liquid boundary. The angle of the contact for pure water and clean glass is zero but for ordinary water and glass it is about 18c. in general the angle of contact is acute (less than 90c) in the case of liquids which wet the surface of the solid. The angle of contact between mercury and glass is 135c. in general the angle of contact is obtuse (more than 90c) in the case of a liquid which does not wet the surface of the solid. The shape of a liquid drop on a solid surface depends on surface tension and also angle of contact.





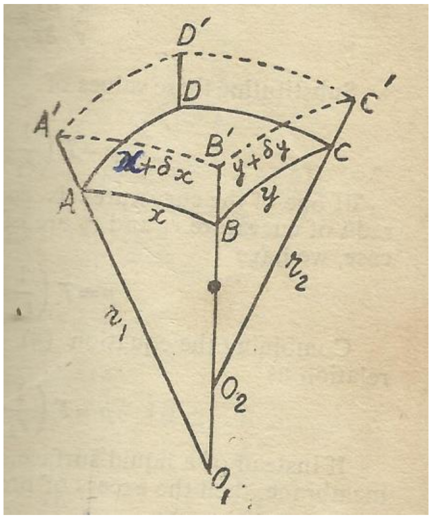
Pressure difference across a curved surface



When the free surface of a liquid is a plane as in fig1, a molecule in the surface is attracted by other liquid molecules equally in all directions consequently. The resultant force due to surface tension is zero. But if the liquid surface is curved, there is a resultant force of surface. For a convex liquid surface fig2. This resultant force is directed inwards towards the interior of the liquid surface (fig 3) for a concave liq surface (fig 3). It acts outwards away from the surface.

Hence, for the equilibrium of a curved surface, there must be pressure difference across it and then the resultant force due to surface tension will be balanced by the excess of pressure force, acting on the concave side.

Expression for excess pressure on a curved surface [pressure difference]



If we have a curved liquid surface at rest, then the inward pressure on it due to S.T. must be balanced by an equal excess of pressure outward, acting on the concave side.

Let ABCD be a small curvilinear rectangle of the curved liquid surface. Its side AB is of length x and radius of curvature r_1 with centre at o, and the side BC is of length ‘ y ‘ radius of curvature r2 with centre o2 clearly $AO_1 = BO_1 = r_1 And BO_2 = CO_2 = r_2$ Geometrically radii of curvature such as AO1 and BO2 are called principle radii of curvature. Area of the rectangle ABCD = xy

Let the excess of pressure on the concave side be P. when the liquid surface is at rest the outward force on the element
ABCD= pxy

Suppose the surface is expanded by giving an infinitesimally small normal displacement δz so that the element occupies a new position $A^1B^1C^1D^1$. Hence the work done by the excess pressure P is.

W = force X displacement

$$= pxy \times \delta z \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (1)$$

If $x + \delta x And y + \delta y$ be the lengths $A^1B^1 And B^1C^1$ respectively, then increase in the area of the liquid surface under consideration Is

$$= (x + \delta x)(y + \delta y) - xy \; = x\delta y + y\delta x$$

The product $\delta x \quad \delta y$ of very small quantities has been neglected.

*Increase in the surface energy = surface tension X Increase in area

$$=T(x\delta y + y\delta x)..................................(2)$$

This increase in the surface energy is equal to the work done in expanding the surface excess of pressure, hence equating

(1) And (2)

We get

P xy $\delta z = T(x\delta y + y\delta x)$

OR $P = T\left(\frac{1}{y}.\frac{\delta y}{\delta z} + \frac{1}{x}\frac{\delta x}{\delta z}\right)$.....................(3)

Now from similar triangle $ABO_1 And A^1B^1O_1$

We have

$$\frac{A^1B^1}{A^1O_1} = \frac{AB}{AO_1} \quad \textbf{or} \quad \frac{X+\delta X}{r_1+\delta z} = \frac{x}{r_1}$$

$$\left[\because A^1O_1 = AO_1 + AA^1 = r_1 + \delta_2\right]$$

OR $\frac{x+\delta x}{x} = \frac{r_1+\delta_2}{r_1}$ Or $1+\frac{\delta x}{x} = 1+\frac{\delta z}{r_1}$

Or $\frac{\delta x}{x} = \frac{\delta z}{r_1}$ $\therefore \frac{1}{x}\frac{\delta x}{\delta z} = \frac{1}{r_1}$

Similarly from similar triangles BCO2 and $B^1C^1O_2$ we have

$$\frac{1}{y}.\frac{\delta y}{\delta z} = \frac{1}{r_2}$$

Substituting these values of $\frac{1}{x}\frac{\delta x}{\delta z} and \frac{1}{y}\frac{\delta y}{\delta z}$ in eqn (3)

We get

$$P = T\left(\frac{1}{r_1} + \frac{1}{r_2}\right).....................(4)$$

if one of the curvature is convex and the other is concave, the radii of curvature r1 and r2 are of opposite signs thus in such a case we have.

$$P = T\left[\frac{1}{r_1} - \frac{1}{r_2}\right].....................(5)$$

Combining the equations 4 and 5 we may write the general relation as

$$P = T\left[\frac{1}{r_1} \pm \frac{1}{r_2}\right]............................(6)$$

If instead of a liquid surface, there are two surfaces of a film or membrane, then the excess of pressure is given by.

$$P = 2T\left[\frac{1}{r_1} \pm \frac{1}{r_2}\right]..................(7)$$

The relation 6 and 7 hold for all surface. A few important particular cases are given below.

1. Spherical surface – it has two surfaces with negligible thickness and r1 =r2=r

[In case of spherical surface cylindrical bubble :- a) In case of a single spherical surface such as that of a liquid drop or an air bubble inside the liquid.

We have $r_1 = r_2 = r(say)$

Hence $P = T\left(\frac{1}{r} + \frac{1}{r}\right) = \frac{2T}{r}$

b) In case of a spherical film, which has two surface such as a soap bubble, the expression for excess pressure is.

$$P = 2 \times \frac{2T}{r} = \frac{4T}{r}$$

2. Case of cylindrical surface: if the surface is cylindrical, one radius of curvature is infinite and the other is equal to the radius of the cylinder, so that for a cylindrical drop of a liq or a cylindrical bubbles in liquid.

$$P = \frac{T}{r}$$

And for a hollow cylindrical film [for two surfaces]

We have

$$P = \frac{2T}{r}$$

3. Case of catenoid: if the surface is one of revolution with no difference of pressure, the surface is catenoid, Here p=o hence

we have

$$\frac{1}{r_1} \pm \frac{1}{r_2} = o$$

An example of such a surface is that of a soap film, supported in between two parallel rings and the ends of the film are burst so that

P = O

[This is the case of a soap film supported in between two parallel rings with two of its ends open to the atmosphere]

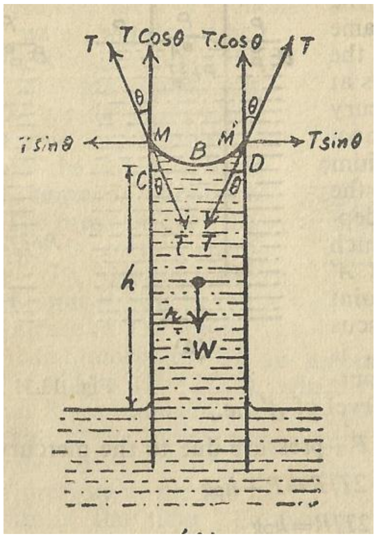
Capillarity: -

A tube of very fine bore is called a capillary tube. When one end of a capillary tube is dipped in water, then water level in the capillary tube rises above the outside level of the water. On the other hand if one end of the capillary tube is dipped in mercury, the mercury level in the capillary tube falls below the outside level of mercury. In general a liquid which wets the tube rises and a liquid which does not wet the tube falls in the tube [less the diameter of the bore, more is the rise or fall of liquid]. This phenomenon of rise or fall of a liquid in a tube of fine bore above or below the outside level of the liq is called capillary.

Some applications of capillary.

1. In an oil lamp, the oil rises up the wick on account of capillary
2. A blotting paper sucks ink on account of capillary
3. S ap rises from the roots thro the stem of a free on account of capillary

Capillarity- rise of liquid in a capillary tube



The rise of liquid in a capillary tube is one of the most important effects of S.T. A tube with a fine bore is known as capillary tube and is so named from the Latin word cap illus. If a capillary tube is dipped in a liquid which wets it, the liquid immediately rises in the tube. If the tube is not very narrow and the angle of contact is zero then the forces acting on the liquid in the tube are the upward force due to surface tension reaction. The vertical component of which is T$Cos\theta$ and acts along the liquid glass interfere in a circle so that the total upward force due to it is $2\pi rT\cos\theta$, where θ is the angle of contact.

This force supports the column 'h' of the liquid. The column is cylindrical almost along the whole length but there is a small volume of the liquid in the meniscus to be taken into account.

This is = $\pi r^2 \times r - \frac{2}{3}\pi r^3 = \frac{1}{3}\pi r^3$

So that the total volume of the liquid supported by the S.T forces.

$$\pi r^2 h + \frac{1}{3}\pi r^3 = \pi r^2\left(h + \frac{r}{3}\right)$$

Its weight = $\pi r^2\left(h + \frac{r}{3}\right)\rho g$

Therefore, for equilibrium $2\pi r \times T\cos\theta = \pi r^2\left(h + \frac{r}{3}\right)\rho g$

Or $\left(h + \frac{r}{3}\right) = \frac{2T\cos\theta}{rpg}$

For narrow tubes $\frac{r}{3}$ can be neglected in comparisons of 'h'

$$h = \frac{2T\cos\theta}{r\rho g}$$

For liquids (e.g. water) which wet the glass the angle of contact practically zero (i.e.Practically zero (i.e. $\cos\theta$ =1)

Then $h = \frac{2T}{r\rho g}$

Knowing the density 'p' of the liquid and measuring the values of r and h with the half of a venire microscope, the S.T of a liq can be determined in laboratory.

Tube of insufficient length

We have deduced above that a liquid in a capillary tube rises to a max height h given by the relation

$$h = \frac{2T\cos\theta}{r\rho g}$$

If 'R' is the radius of curvature of the meniscus then $r = R\cos\theta$

$$\therefore h = \frac{2T\cos\theta}{R\cos\theta \rho g} = \frac{2T}{R\rho g}$$

OR $RH = \frac{2T}{\rho g} = const$

When the length of the tube is greater than 'h' the radius of curvature of the liq meniscus remains const and it is the height of the liq which adjust itself until the above equation is satisfied.

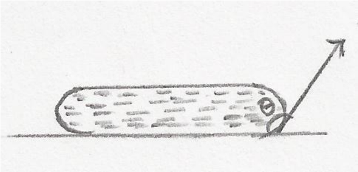
But if the length of the tube (= h1) is less than h the required length of the liquid column, the only variable is R. the liquid rises to the top and there forms a new surface (which is concave upward) whose radius curvature R, is greater than R so that R1h1= Rh = constant

Angle of contact remaining the same, the radius of curvature of the meniscus increases.

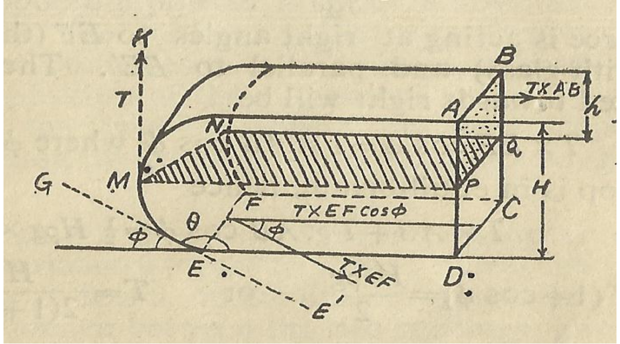
Qn. Define surface tension and angle of contact. Derive an expression for the rise of liquid in a capillary tube, (of insufficient length)

Quinke's method [Determination of surface tension]

This method is applicable in the case of liquids which do not wet the surface in contact with them, as for example mercury. We shall consider here the case of mercury for which is so frequently used.



Consider a drop of liquid on flat surface of the solid. If a liquid does not wet a solid a small drop of it resting on the solid surface tension. As the size of the drop is increased force of gravity dominates and the drop flattens out its top becomes perfectly horizontal. The drop then takes up the shape as shown in figure above.



Let us imagine a large drop of mercury which has been cut into two halves by a vertical plane ABCD, passing through its centre and Perpendicular to its length. Imagine that one half is again cut by two vertical planes BCEF and ADGK normal to ABCD. In this way we get a thin slice of the drop having parallel vertical faces and horizontal with AB. If MN is the most bulging out part of the drop, the tangent plane MK at MN is obviously vertical and the horizontal plane MNOP in the drop is the plane of maximum area.

Let us consider the equilibrium of the portion of the slice above the plane MNOP. The various forces acting on the slice area.

1. The Pull due to surface tension T acting Perpendicularly towards the right its magnitude is T x AB
2. The force due to hydrostatic pressure over the plane face ABOP acting towards the left.

The hydrostatic pressure is zero at AB and increase to hpg at PO

Where, h=AP=BO and ρ= Density of mercury

Therefore

Average hydrostatic pressure $= \frac{o + h\rho g}{2}$

$$= \frac{h\rho g}{2}$$

Now

Average hydrostatic force on ABOP

= pressure x area ABOP

$= \frac{h\rho g}{2} \times AB \times h$

3. Surface tension acting vertically along the line MK. It has no component in the horizontal plane.

Since slice is in equilibrium the horizontal force 1 and 2 must balance each other.

$$i.e. \quad T \times AB = \frac{h\rho g}{2}.AB \times h$$

$$\therefore T = \frac{h^2 \rho g}{2}$$

Hence by measuring ‘h’ the distance of the most bulging out part of the drop from the horizontal top. We can determine the value of surface tension.

Qn: - Describe with relevant theory Quinke’s method to determine surface tension of mercury.
(10-marks)

Variation of surface tension with temperature

The Surface tension of a liquid decrease with the increase of temperature. In the case of water its surface tension decrease at the case of water its surface tension decrease at the rate of 0.14 dynes per 12C rise of temperature. For a small range of temperature the relation is linear and given by

$$T = T_o(1 - \alpha t)$$

Where T is the surface tension at $1^0 C$ and To at 0^0 C and α is the temperature coefficient of surface tension

The surface tension reduces to zero at critical temperature because at that temperature the interface between the liquid and vapour disappears. The best relation connecting S.T. and temperature is due to Eotvos and later modified by Ramsay and shields and is given by

$$T[MVX]^{3/2} - K(\theta_C - \theta - d)$$

Where M is the molecular weight of the liquid and V its specific volume. T is the surface tension at Q absolute, Qc is the critical temperature, X – coefficient of association of the liquid at 0c, land k are constants.

This shows that the S.T is zero when Q = Qc – d at temperature a little below the critical temperature.

Effect of Impurities on Surface Tension

If the impurity present in a liquid is completely soluble in the liquid, its surface tension increases. For example, on dissolving salt in water, its surface tension increases.

If the impurity present in a liquid is partially soluble in the liquid, its surface tension decreases. For example, on maxing detergent in water, its surface tension decreases.

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B. V. V. Sangha’s
BASAVESHWAR SCIENCE COLLEGE, BAGALKOT
DEPARTMENT OF PHYSICS

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Unit-3: Molecular & LASER Physics **Name:** Prof. (Smt.) V. N. Vanakudure

Course Code: 21BSC5C5PHY2L

RAMAN EFFECT

INTRODUCTION

When sun light passes through the atmosphere, it is absorbed by the molecules in the atmosphere and then reradiated in all directions. This is known as Scattering of light. There are two types of scattering of light- Coherent and Incoherent scattering.

COHERENTSCATTERING:

When light is incident on certain substances, it gets scattered. If the scattered radiation has the same wavelength as that of incident radiation, the scattering is said to be coherent.

During coherent scattering, there is no absorption of light energy by the medium. Coherent scattering is also known as elastic scattering or Rayleigh scattering.

INCOHERENTSCATTERING:

When light is incident on certain substance, it gets scattered and if the scattered radiation has the different wavelength or different wavelengths than that of incident radiation, then scattering is said to be incoherent. During incoherent scattering, the scattering medium absorbs some amount of incident light energy. Incoherent scattering is also known as Inelastic scattering or Stokes scattering.

RAYLEIGH’SSCATTERING:

Rayleigh showed theoretically that the intensity of scattered light is inversely proportional to the fourth power of the wavelength. i.e I/λ^4This is known as Rayleigh’s law of scattering.

RAMAN EFFECT

In 1928 C. R. Raman experimentally found that when a beam of monochromatic light was passed through organic substance such as benzene, toluene etc… The scattered light contains some new frequencies in addition to that ofthe incident light. It isknown as Raman Effect.

Raman used a very simple apparatus consisting of a round bottom flask filled with dust free benzene and it was strongly illuminated by the 4358 X 10^{-10} m {4358A^0} light from the mercury are suitably filtered & concentrate by a lens.

The scattered light was examined by means of a spectroscope placed transversely. i.e in the direction at right angles to that of the incident radiation.

On observation it was found that in the scattered light, there were number of new lines on either sides of the original one. The lines having frequencies smaller than that of the incident frequency are called Stokes lines. And those having greater frequencies are called Anti-stokes lines. The observed spectrum is known as Raman spectrum. And the known as Raman lines.

If $V_0$is the frequency of the incident light and Vs is that of the scattered light, then the Raman shift ΔV is given by $\Delta V=V_0\sim$ Vs. Raman shift does not depend on the frequency of the incident light but it depends upon the nature of scattering substance. Thus Raman shiftisthecharacteristicofscatteringsubstance.ForstokeslinesΔVis+veandforAnti-stokeslines ΔVis–ve.

The difference between Rayleigh scattering and Ramanscattering is that in the former, the frequency of the scattered light is always equal to that of the incident light where as in the Raman scattering, in addition to the frequency of the incident light, some new frequencies are present. Thus Raman Effect is called in coherent scattering and is considered as the optical analogue of the Compton Effect. As we know Rayleigh scattering is known as coherent scattering.

Experimental study of Raman Effect

The apparatus shown in figure, first developed by Wood, is used for studying Raman Effect in liquids. It consists of glass tube 'AB' containing the pure experimental liquid free from dust and air bubbles, the tube is closed at one end by an optically plane glass plate 'W' and at the other end it is drown into a horn (H) and blackened on the outside.

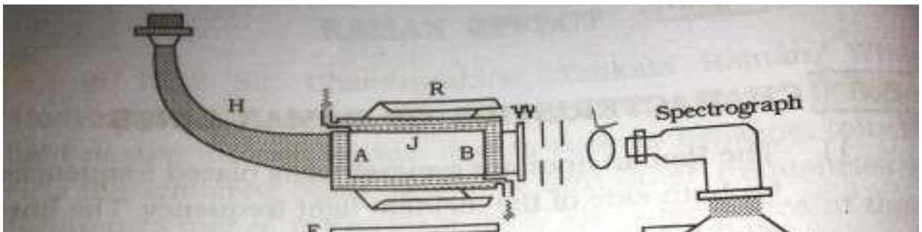


Fig. (1)

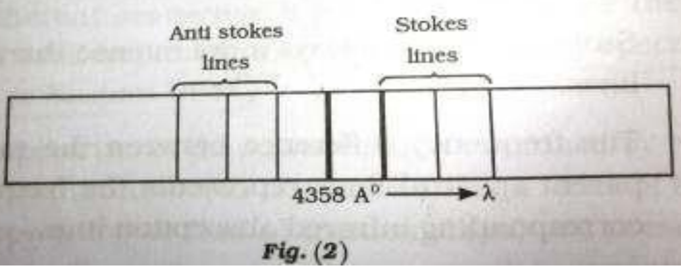


Fig. (2)

Light from a mercury are ‘S’ is passed through a filter ‘F’ which allows only monochromatic radiation of λ=4358A^0 to passed through it. The tube is surrounded by water-jacket (J) through which water is circulated to prevent over heating of the liquid. A semi cylindrical aluminum reflector ‘R’ is used to increase the intensity of illumination. The scattered light coming out of ‘W’ is condensed, on the slit of a spectrograph. The spectrograph must have a large light gathering power and the prism must have a large resolving power. Short focus camera is used to photograph the spectrum.

On developing the photographic plate it exhibits a number of stokes lines a few antis-stokes lines and a strong unified line.

CHARACTERISTICSOF RAMAN LINES

1. Thestokeslinesare always moreintensethananti-stokes lines.
2. TheRamanlinesaresymmetricallydisplacedabouttheparent line.
3. The frequency difference between the modified and parent line presents the frequency of the corresponding infrared absorption line.

QUANTUMTHEORYOF RAMANEFFECT

Raman Effect is due to interaction between a light photon and a molecule of the scatter. Suppose a photon of frequency v_1 is incident on molecule and there is a collision between the two molecules.

Let m=mass of the molecule, v_1& $v_2$its velocities before and after impact, E_1& E_2 the intrinsic energies of the molecule before and after collision. Let v_2 be the frequency of the scattered photon, applying the principle of conservation of energy

$$E_2+(1/2)mv_2^2+hv_2=E_1+(1/2)mv_1^2+hv_1 \text{--} (1)$$

WemayassumethattheKEofthemoleculeisunalteredduring the process. Hence

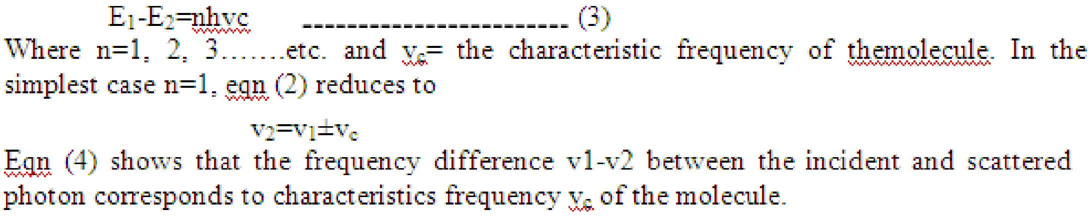
$$E_2+hv_2=E_1+hv_1$$

$$v2- v1=(E1-E2)/h$$

$$v_2=v_1+(E_1-E_2)/h (2)$$

Thereare3cases:

1. When there is no change in the energy of the molecule, $E_1=E_2$ then $v_1= v_2$This represents the unmodified line.
2. If $E_2>E_1$, then $v_2<v_1$, this represents stokes line. It means that the molecule has absorbed some energy from the incident photon. Consequently the scattered photon has lower energy or longer wavelength.
3. If $E_2<E_1$, than $v_2>v_1$ this represents the anti-stokes lines. It means that the molecule was previously in the excited state and it handed over some of its intrinsic energy to incident photon. The scattered photon thus has greater energy or shorter wavelength.



$$E_1\text{-}E_2=nhvc \text{ ------------------------- } (3)$$

Where n=1, 2, 3…….etc. and v_c= the characteristic frequency of themolecule. In the simplest case n=1, eqn (2) reduces to

$$v_2=v_1\pm v_c$$

Eqn (4) shows that the frequency difference v1-v2 between the incident and scattered photon corresponds to characteristics frequency v_c of the molecule.

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B. V. V. Sangha's

BASAVESHWAR SCIENCE COLLEGE, BAGALKOT

DEPARTMENT OF PHYSICS

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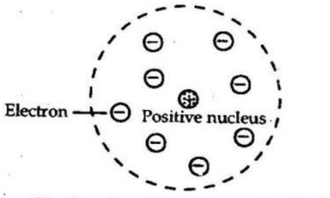
Unit-1: ATOMIC MODELS **Name:** Sri. B. M. Karidyavannavar

Course Code: 21BSC5C5PHY2L

UNIT-1
ATOMIC MODELS



Rutherford's Nuclear atom

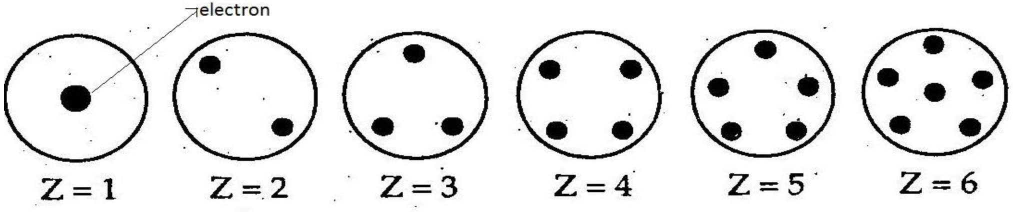
INTRODUCTION:

In nineteenth century, electron was first discovered by J.J. Thomson. It is negatively charged particle. But the atom as a whole is electrically neutral. Hence it is clear that the atom must contain +vely charged particle to balance the negative charge of the electron. This was confirmed by the discovery of the proton. Thomson measured the ratio of e/m value. The charge of electron was measured by Millikan oil drop experiment. The mass of the electron is found by dividing charge e by the ratio e/m. Thomson showed that the mass of the electron is of the order 1/2000th of mass of hydrogen. But they do not know how the +ve and –ve charges are distributed in an atom.

Scientists proposed several theories from time to time regarding the atomic structure. They are
(1) Thomson's plum pudding model.
(2) Rutherford's nuclear model.
(3) Bhor's model.
(4) Sommerfield's relativistic model
(5) Vector model and
(6) Wave mechanical model.

(1) THOMSON'S PLUM-PUDDING MODEL:

According to Thomson the +ve charge inside an atom is uniformly distributed through out the entire atom. The negatively charged electrons were imagined to be embedded at different places inside the continuous +ve charge as shown in the figure.



Thomson's plum - pudding model of stable atoms

DRAW BACKS: According to Thomson, the emission of radiation occurs when the stable distribution of electrons is disturbed and electrons start vibrating like oscillators. Hence emission spectrum consists of a single line of 1400A^o.But we know that the atomic spectra of hydrogen consists of several lines.

(2) RUTHERFORD'S NUCLEAR MODEL:

According to Rutherford's model the atom consists of a tiny massive, +vely charged nucleus surrounded at a relatively great distance by electrons as shown in the figure (from the experiment scattering of alpha particles by thin metal foil).In this model the electrons can’t remain stationary because of the electrostatic force of attraction by the positively charged nucleus. Hence the electrons were revolving around the nucleus. The electrostatic force of attraction provides necessary centripetal force for revolving of electrons. Hence there exist dynamically stable orbits.

DRAW BACKS: Here there is no restriction about the radius of the electron orbit. According to classical electromagnetic theory any charged particle having accelerated motion must emit energy radiation. Hence the electron should radiate energy continuously .so the electron looses energy and spirals down and crashes in to the nucleus within 10^{-8} s .This gives continuous spectrum but not line spectrum.

(3) BHOR’S THEORY:

Inorder to overcome the problem of instability of Rutherford’s planetary model of atom, Bhor proposed that an electron revolving in an orbit such that its angular momentum is quantalised will not radiate energy and the orbit will be stable. If the electron moves from one orbit to another orbit then it emits or absorbs radiation.

DRAW BACKS OF BHOR’S THEORY:

(1) The theory could not explain the spectra of atoms more complex than hydrogen.
(2) The theory does not give any information regarding the distribution and arrangement of electron in an atom.
(3) The theory does not explain the experimentally observed variations in intensity of the spectral lines of an element.
(4) This theory can’t be used to calculate about transitions from one level to another.
(5) This theory can’t be used for the quantitative explanation of chemical bonding.
(6) The theory fails to give correct result when an electric or magnetic field is applied to the atom.
(7) It failed to explain the fine structure of spectral lines.

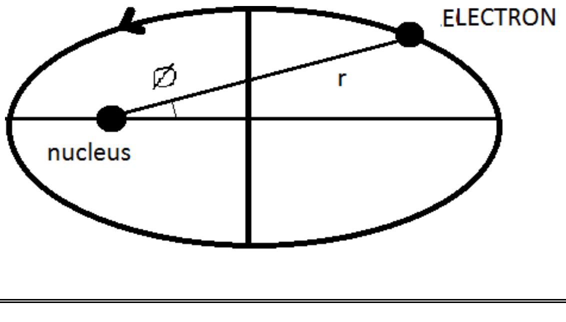
According to Bhor’s theory of circular orbit, we get only a single line when electron jumps from a higher orbit to a lower orbit but experimental results showed that the H_α , H_β , H_γ lines of hydrogen atomic spectra are not single lines. For example H_α consists of five lines. This is called fine structure of spectral line.

(4) SOMMERFELD’S RELATIVISTIC MODEL:

In 1921 sommerfeld modified Bhor’s model by introducing the idea of “motion of electron in an elliptical orbits and taking into consideration the variation of mass with velocity”.

ELLIPTICAL ORBIT:

According to sommerfeld, the electron moving around the nucleus in an elliptical orbit with the nucleus at one focus.In the elliptical orbit the position of the electron at any time may be fixed by two co-ordinates r and ϕ where r is



the radius vector and ϕ is the angle between the radius vector and the major axis of the ellipse which is called azimuthal angle. Consider an electron of mass m and linear tangential velocity v revolving in the elliptical orbit. The tangential velocity of the electron can be resolved into two components. One along the radius vector called radial velocity and the perpendicular to radius vector called the transverse velocity. Corresponding to those velocities the electron has two momenta called as radial momentum and the transverse momentum or azimuthal momentum. Sommerfeld introduced the two quantum numbers $n_r and\ n_\phi$ called as radial quantum numbers and azimuthal quantum numbers. Here $n_r + n_\phi = n$, where n is called principal quantum number.

Corresponding to n=1 there are two possibilities i.e., $n_r = 0, n_\phi = 1 and n_r = 1, n_\phi = 0$.when $n_\phi = 0$ the ellipse is converted into a straight line and the electron pass through the nucleus twice during every period. This type of motion is not possible. Hence, the lowest possible value of $n_\phi = 1$.

Therefore if n = 1 then $n_\phi = 1$[s orbit]

If n = 2 then [p orbit]

$$n_\phi = 2 \qquad (circularorbit)$$

$$n_\phi = 1 \qquad (ellipse)$$

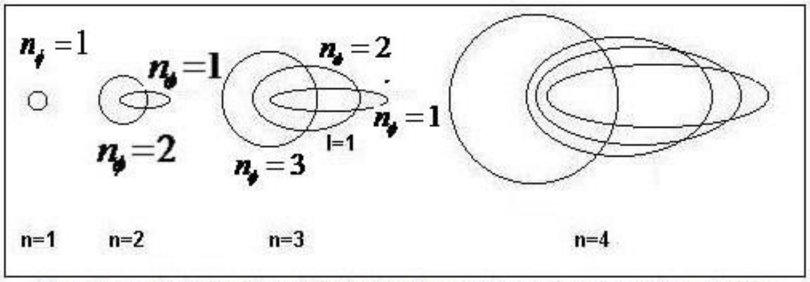
If n = 3 then [d orbit]

$$n_\phi = 3 \qquad (circularorbit\ )$$

$$n_\phi = 2 \qquad (ellipse\ )$$

$$n_\phi = 1 \qquad (ellipse)$$

These are shown in the figure.



The allowed electronic orbits for the four main quantum numbers by the Bohr-Sommerfeld model.

According to sommerfeld each momentum component is separately quantized as

$$\oint P_r dr = n_r h$$

$$\oint P_\phi d\phi = n_\phi h$$

Where, $P_r and P_\phi$ are the components of linear momentum P of the electron along radial direction and transverse direction. $n_r and n_\phi$ are the integers, and $\oint$ indicates that the integration is to be carried over one period of the motion.

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BASAVESHWAR SCIENCE COLLEGE, BAGALKOT
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Unit-3: General Properties of Nuclei　　**Name:** Sri. Husenappa V.

Course Code: 21BSC6C6PHY1L

Unit III

General Properties of Nuclei

SYLLABUS: Nuclear Structure: General Properties of Nuclei, Mass defect, Binding energy; Nuclear forces: Characteristics of nuclear forces- Yukawa's meson theory; Nuclear Models: Liquid drop model, The Shell model, Magic numbers; Nuclear Radiation detectors: G.M. Counter, Cloud chamber, Solid State detector; Elementary Particles: Elementary Particles and their classification

INTRODUCTION: From the scattering of α particles, Rutherford concluded that the atom of any element consists of central core called nucleus and electrons moving around it. The entire mass of the atom and positive charge is concentrated inside the nucleus.

Mass of electron=9.1×10^{-31}kg
Mass of Proton=1.673×10^{-27}kg
Mass of Neutron=1.674×10^{-27} kg

The number of protons in the nucleus is called atomic number and the sum of protons and neutrons is called as mass number. The stability of the nucleus depends upon the relative number of protons and neutrons.

BASIC PROPERTIES OF NUCLEUS:

(a) NUCLEAR MASS:

The mass of the nucleus is the sum of the masses of the neutrons and protons. It is expressed in terms of atomic mass unit

1 a.m.u=1.66×10^{-27}kg=9.315MeV

EX: mass of ${}_6C^{12}$ is 12 a.m.u

Mass of the nucleus $=Zm_p+Nm_n$　　where m_p=mass of proton
Real nuclear mass< Zm_p+Nm_n　　m_n=mass of neutron

The difference of the mss is called mass defect. The mass defect is converted into energy according to $E=mc^2$ formula.

(b) NUCLEAR CHARGE:

The charge on the nucleus is due to protons contained in it. The charge on each proton is $+1.6\times10^{-19}$ coulomb. This is equal in magnitude to the charge of an electron. For example, a hydrogen nucleus carries a single unit charge.,

(c) NUCLEAR RADIUS:

Nuclear diameter can be determined by the experiments like scattering of fast protons or neutrons or scattering of high energy of electrons. Rutherford concluded that the distance of the closest approach of the α particle to the nucleus of the scatter can be regarded as a measure of the size of the nucleus. He found this distance of the order of 10^{-14}m. This can be determined from the empirical formula

$$r=r_oA^{1/3}$$

Where r_o=linear constant 1.4×10^{-15}m
` A= mass of the nucleus.

EX :(1) Carbon (A=12) : $r=1.4\times10^{-15}\times(12)^{1/3}=3.21\times10^{-15}$m

(2) Copper (A=63) : $r=1.4\times10^{-15}(63)^{1/3}=5.97\times10^{-15}$m

(3) Uranium (A=238): $r=8.68\times10^{-15}$m

NUCLEAR DENSITY:

Density of Nucleus =mass of the Nucleus/volume of the Nucleus

= (mass number x mass of proton)/ $\frac{4}{3}\pi r^3$

$$= \frac{AX1.673X\,10^{-27}}{\frac{4}{3}\pi\left(1.5X\,10^{-15}\,A^{\frac{1}{3}}\right)^3}$$

$$= \frac{1.673X10^{-2}\,A}{14.15X10^{-45}\,A} = 1.18x10^{17}\,kg/m^3$$

NUCLEAR QUANTUM STATES:

Every nucleus possesses a set of quantum states in a corresponding number of discrete energy levels. Transition between different nuclear states is accompanied by the emission of γ rays.

NUCLEAR SPIN:

In atomic spectra, we found many spectral lines which have fine structure. That was explained by electron spin. Many of these fine structure lines show still finer structure called “hyper fine structure” which has been attribute to the nuclear spin.

Both the proton and the neutron have an intrinsic angular momentum generally it is called as its spin.

The magnitude of the spin angular momentum is $\frac{1}{2}\hbar$ where $\hbar = \frac{h}{2\pi}$. The nucleons [protons and neutrons] possess orbital angular momentum due to motion about the centre of the nucleus. The resultant angular momentum I of the nucleon is obtained by adding spin and orbital angular momentum of all nucleons in the nucleus.

Total angular momentum I =L+S

Where L=orbital angular momentum

S=spin angular momentum

MAGNETIC DIPOLE MOMENT OF NUCLEI (μ):

We know that the charged particle moving in a closed path produces a magnetic field. The spinning electron is associated with a magnetic dipole moment of one “Bhor magneton”

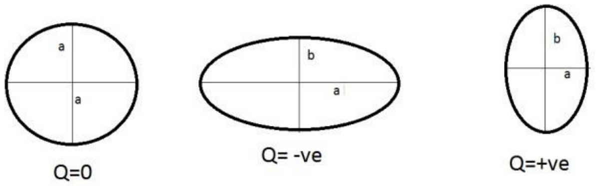
i.e., $\mu_e = \frac{e\hbar}{2m_e}$ where e is the charge m_e is the mass of the electron.

Due to proton spin, it has Magnetic dipole moment $\mu_N = \frac{e\hbar}{2m_p}$ where m_p is the proton mass and μ_N is called nuclear magneton.

Since m_p=1836xm_e so nuclear magneton $\frac{1}{1836}$ of a Bohr magneton.

Neutron is a neutral particle. So it is very difficult to understand how it can have a magnetic moment. It is found that neutron has a magnetic moment $\mu_n = -1.9128\mu_N$. To explain μ_n, it was assumed that neutron contains equal amount of +ve and –ve charges. If these charges are not uniformly distributed then a spin magnetic moment may arise. The magnetic moments of nuclei are found to vary between -2 to +4 nuclear magneton.

ELECTRIC QUADRUPOLE MOMENT (Q): Experiments show that the shape of the nucleus is not spherical but it is an ellipsoid of revolution. The derivation from the spherical symmetry is measured by a quantity called its electric quadrupole moment.



SHAPE OF NUCLEUS AND ELECTRIC QUADRUPOLE MOMENTS

If the axis of symmetry is 2a and the diameter in the perpendicular direction is 2b, the electric quadrupole moment is defined as

$$Q=\frac{2}{5}ze\left(b^{2}-a^{2}\right)$$

Where z is atomic number and Ze is total charge of nucleus.

Therefore Q = 0 for spherical shaped nucleus, Q is negative for a > b and Q is positive for b > a as shown in the above fig.

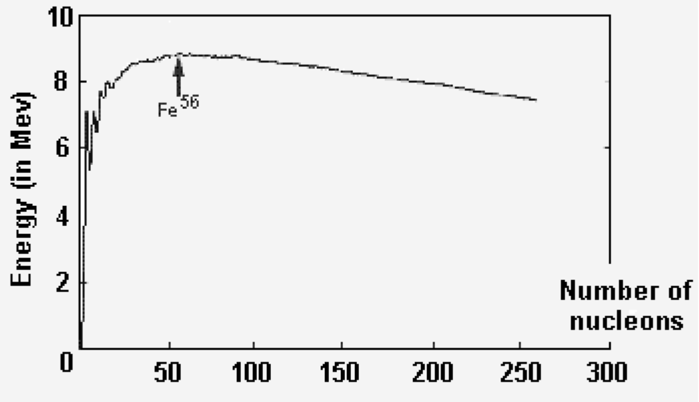
BINDING ENERGY OF NUCLEUS:

When protons and neutrons combine to form a nucleus, some of the mass (Δm) is found to be disappeared. This is known as mass defect. This Δm mass is converted into an amount of energy equal to $(\Delta m)c^2$. This energy is called the binding energy of the nucleus. To separate a stable nucleus into its constituent protons and neutrons, the minimum energy required is the binding energy. If the binding energy is large the nucleus is stable.

If M is the mass of the nucleus having Z protons and N neutrons then

$B.E= [(Zm_p+Nm_n)-M]\, c^2$

Where, m_p and m_n are the mass of proton and neutron respectively. If B.E<0, the nucleus is unstable and it will disintegrate by itself.



The ratio of binding energy of the nucleus and number of nucleons in it is known as B.E per nucleon. The B.E per nucleon is plotted as function of mass number A in the above fig. from the graph it is clear that nuclei of intermediate mass[A=40 to 140] are most stable nuclei. The binding energies of He^4, C^{12}, O^{16} are considerably greater than those of their neighbors.

When a heavier nucleus splits into lighter nuclei or lighter nuclei join to form heavier nucleus energy is released. The first process is called nuclear fission and the second is called nuclear fusion.

BINDING ENERGY OF DEUTRON:

The isotopes of hydrogen are ${}_1H^1$ and ${}_1H^2$. The heaviest isotope of hydrogen is called deuteron. It consists of one proton and one neutron in its nucleus.

B.E of ${}_1H^2$ =total mass of proton and neutron-actual mass of ${}_1H^2$

B.E of $_1H^2$ = (2.016490-2014104)a.m.u
=0.002386x931 MeV
=2.23 MeV

This shows that when a proton and neutron are combined to form a deuteron, energy equal to 2.23 MeV is released.

NUCLEAR MODELS:

The force that binds the proton and the neutron so securely into a tiny molecule is the strongest type of force known. This nucleus force is a short range force. To explain the nuclear properties, theoretical physicist developed various nuclear models. They are (1) liquid drop model and (2) shell model

LIQUID DROP MODEL:

This model was proposed by Neil's Bhor in 1937. According to this model

(1) The nucleus is similar to a small electrically charged liquid drop i.e., nucleus take a spherical shape for its stability.
(2) The nucleons move within this spherical enclosure like molecules in a liquid drop.
(3) The motion of nucleons within nucleus is a measure of nuclear temperature as the molecular motion of molecules in liquid is the measure of its temperature.
(4) The nucleons always remains constant distant a part and share among them the total energy of the nucleus.
(5) The nucleons inside the nucleus are attracted from all sides by neighboring nucleons while those on the surface are attracted from one side only. In this way the binding energy for the nucleons at the surface of the nucleus is smaller than the binding energy for the nucleons inside the nucleus.

In this model the nucleus is regarded as arranged to a drop of liquid. Hence this model is known as liquid drop model.

FOLLOWING ARE THE ANALOGIES BETWEEN LIQUID DROP AND A NUCLEUS:

(1) Both are spherical in nature.
(2) In both the cases, the density is independent of its volume.
(3) The molecules in liquid drop interact over short ranges and so is true for nucleons in nucleus.
(4) As the surface tension forces act on the surface of a drop similarly a potential barrier acts on the surface of nucleus.
(5) When the temperature of the molecules in a liquid drop increased, evaporation of molecules takes place. Similarly, when the nucleons in the nucleus are subjected to external energy, a compound nucleus is formed which emits nucleons almost immediately.

MERITS:

(1) It has been successfully explains nuclear reactions and nuclear fission.
(2) The calculations of atomic mass and binding energy can be done with good accuracy.

DE-MERITS:

This model fails to explain other properties like magic numbers (2, 8, 20, 28, 50, and 82,126).

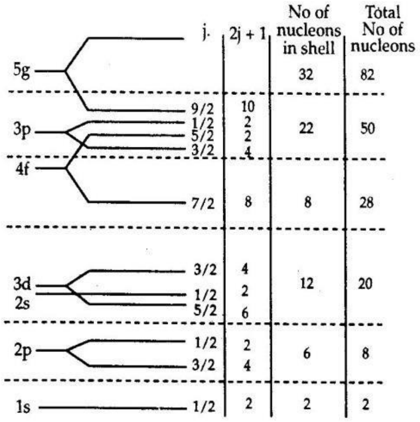
THE SHELLMODEL:

The nucleus consists of a series of protons and neutrons placed in certain discrete levels or shells just like the electrons in the discrete shells of an atom. According to Pauli's exclusion principle two protons with opposite spins and two neutrons having opposite spins are accommodated in a particular shell. In this way the first shell accommodates two protons and two neutrons and is more tightly bound than other shells.

THE CONCEPT OF THE SHELL MODEL IS BASED ON THE FOLLOWING FACT:

It has been observed that the nuclei containing protons and neutrons numbers 2, 8,20,50,82,126 called magic numbers are exceptionally stable. This shows that there are definite energy shells in the nuclei.

In 1949 Maria-Mayer and Jensen proposed that magic numbers can be obtained by assuming that there is strong interaction between the spin angular momentum S and the orbital angular momentum L of the nucleon. If we write j=*l* + s. we get two values. They are *l*+s and *l*-s. The energy depends on total angular momentum quantum number j. for each value of j there will be 2j+1 different states corresponding to different projections of j on the Z-axis. Thus there will be 2j+1nucleons in a state of given j.



As shown in the fig, the energy levels are grouped into shells such that each shell contains closely spaced energy levels and two consecutive shells are separated by a large gap. The closed shells are obtained ,whenever the number of nucleons are 2,8,20,28,50 etc… Thus magic numbers are obtained. The shell structure applies to both neutrons and protons separately.

MERITS:

This model explains the magic numbers, observed angular momenta, magnetic moments and quadrupole moments of nuclei.

DE-MERITS:

This model fails to explain the large nuclear quadrupole moment and spherical shapes of many nuclei.

Magic numbers: In nuclear physics, a **magic number** is a number of nucleons (either protons or neutrons, separately) such that they are arranged into complete shells within the atomic nucleus. The seven most widely recognized magic numbers are **2, 8, 20, 28, 50, 82, and 126** .For protons, this corresponds to the elements helium, oxygen, calcium, nickel, tin, lead and the hypothetical element 126 or eka-plutonium, although 126 is so far only known to be a magic number for neutrons. Atomic nuclei consisting of such a magic number of nucleons have a higher average binding energy per nucleon than one would expect based upon predictions such as the semi-empirical mass formula and are hence more stable against nuclear decay.

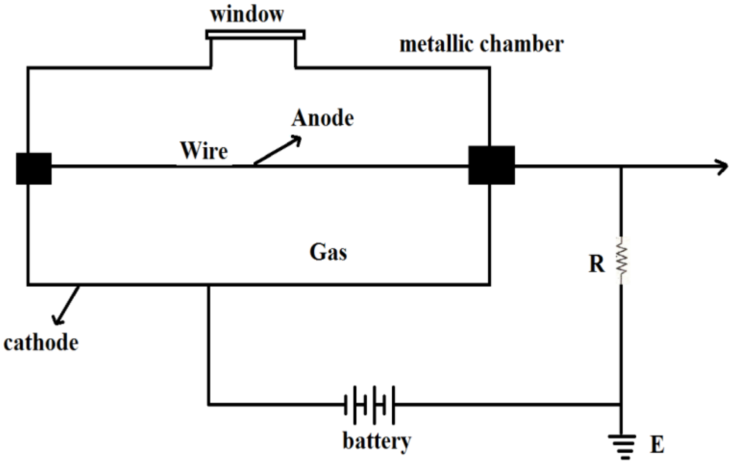
Parity: Parity is a fundamental character of nucleus. Parity can be even or odd depending on nucleon number of the atomic nucleus.

In physics, property important in the quantum-mechanical description of a physical system. In most cases it relates to the symmetry of the wave function representing a system of fundamental particles. A parity transformation replaces such a system with a type of mirror image. Stated mathematically, the spatial coordinates describing the system are inverted through the point at the origin; that is, the coordinates x, y, and z are replaced with $-x$, $-y$, and $-z$. In general, if a system is identical to the original system after a parity transformation, the system is said to have even parity. If the final formulation is the negative of the original, its parity is odd. For either parity the physical observables, which depend on the square of the wave function, are unchanged. A complex system has an overall parity that is the product of the parities of its components.

G.M COUNTER:

DESCRIPITION:

As shown in the fig G.M counter consists of a fine wire of tungsten along the axis of cylinder copper tube. The tube contains a gas at a pressure of about 10cm of Hg. This gas is a mixture of 90% argon and 10% ethyl alcohol. The ionization particles enter into the chamber through mica window. A potential difference of about 800V to 2000V is applied between the copper tube [cathode] and the tungsten wire [anode] by means of a battery. A high resistance R is also connected in series with the battery.



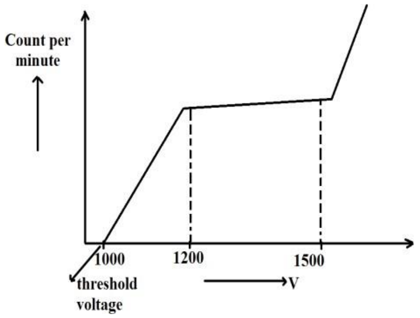
WORKING:

When the charged particle is allowed to pass through the window, it ionizes the gas molecules inside the tube. Hence +vely charged ions and electrons in pairs are produced. The anode attracts the electrons while the cathode attracts the +ve ions. Hence the ionization current is produced and it depends upon the applied voltage. At sufficiently high voltages, the electrons gain high K.E and cause further ionization of argon atoms. Hence large no: of secondary electrons are produced.

The incoming particle serves the purpose of triggering the release of an avalanche of secondary electrons. The electrons quickly reach the anode and produce ionization current. The +ve ion move more slowly away from anode and they form a sheath around the anode for a short while. They reduce the potential difference between the electrodes to very low value. The current therefore stops. In this way brief pulse of current flows through the resistance R. this current creates a potential difference across R. the pulse is amplified and fed to counter circuit. As each incoming particle produces a pulse, hence the no: of particles can be counted.

VOLTAGE CHARACTERISTIC CURRENT:

If we draw a graph by taking voltage on X-axis and count per minute on Y-axis then the graph is as shown in the fig. From the graph it is clear that the current pulses are too small to be detect until the applied voltage reaches the value indicates as the threshold voltage. As the P.D increases the ionization also increases and the pulse rate increase rapidly upto a flat portion called the plateau. In this region count rate



is nearly independent of the P.D .Beyond the plateau, if the voltage is increased a continuous discharge will takes place. This is un-desirable.

QUENCHING: When +ve ions of high K.E reach the walls of the tube, then electron emission takes place from metal cathode. These electrons travel towards the anode and produce un-wanted pulse in a continuous process. The method used to prevent a continuous series of pulses is called Quenching. The self quenching is obtained by adding alcohol vapour inside the tube. Alcohol has low ionization potential. The argon ions on their journey to the cathode are neutralized by acquiring an electron from the alcohol molecules. Now only alcohol ions reach the cathode and become neutral. The K.E of alcohol molecules is used for dissociation of alcohol atoms. Thus it is a self quenching.

In G.M counter the slowly moving +ve ions take about 100 μ s to reach the cathode. This time is known as dead time. If a second particle enters the tube during this time, it will not be recorded as the P.D across the electrodes is very low. After dead time, the tube takes nearly 100 μ s before it regains its original condition. This time interval is known as recovery time. The sum of these two is known as paralysis time. Hence G.M counter can count nearly 500 particles per second.

ADVANTAGES:

(1) This G.M counter is very useful to detect and counting β particles.

(2) It is very useful to study the cosmic rays.

DIS ADVANTAGES:

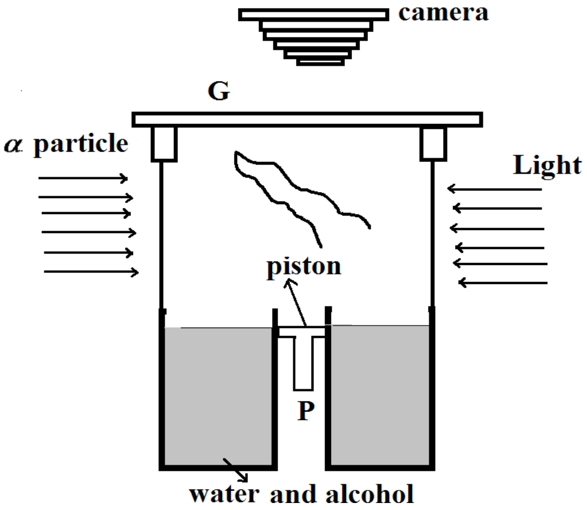
It can’t give information as charge, momentum, energy, range of the particles.

WILSON CLOUD CHAMBER:

In 1931 Wilson designed an instrument known as cloud chamber it is used to detect and record the paths of charged particle.

PRINCIPLE:

If a saturated water vapour undergoes a sudden expansion, then due to cooling the vapour gets super saturated. At this instant of expansion, if an ionizing particle enters the chamber, the ions it produces becomes condensation centers of the molecules of super saturated vapour. By illuminating the chamber, we can record the ion tracks by using camera.



CONSTRUCTION:

The experimental arrangement is as shown in the fig. it consists of an air-tight cylinder C provided with a movable piston P and upper end covered with a glass plate G. the chamber contains a mixture of alcohol vapour and air. A small amount of water and alcohol is kept in a trough at the lower end of the chamber. The chamber is illuminated by mercury vapour lamp. The charged particle like $\alpha or \beta$ rays is allowed to enter the chamber by a side window. A camera is adjusted on the upper side of the chamber.

WORKING: The air inside the chamber is cooled and becomes super saturated by suddenly increasing the volume of the chamber by using piston P. as a result alcohol vapour condenses into drops forms fog in the chamber. When $\alpha or \beta$ rays are allowed to enter in the chamber, they ionize the gas. Now –ve and +ve ions are formed all along the path of these rays. If at the same time expansion takes place, fog drops will be formed on newly created ions. A clear track in the form of drop is thus formed. The drops are clearly visible when the chamber is illuminated by light. The track can be photographed with the help of camera. Immediately after this, the track is removed by applying an electric field across the air gap. Now the chamber gets ready for the next photograph.

ADVANTAGES:

(1) It is used for the study of radioactive radiations.
(2) By counting drops in cloud track, the specific ionization can be determined.
(3) It is used for recording the tracks of ionizing particles.
(4) By seeing the direction of track in the magnetic field, the sign of the ionizing particle can be determined.

DIS-ADVANTAGES:

(1) If the range of the particle exceeds the dimensions of the chamber then the whole track is not photographed.
(2) This cannot directly record the track of electrically neutral particles like neutrons.
(3) It is not continuously sensitive and hence there is a possibility of missing certain nuclear reactions.

SOLID STATE DETECTOR(semiconductor radiation detector)**:** In a semiconductor radiation detector, incident radiation interacts with the detector material, a semiconductor such as Si or Ge, to create hole electron pairs. These pairs are collected by charged electrodes with the electrons migrating to the positive electrode and the holes to the negative electrode, thereby creating an electrical pulse. Such pulses contain information on the type, energy, time of arrival, and number of particles arriving per unit time.

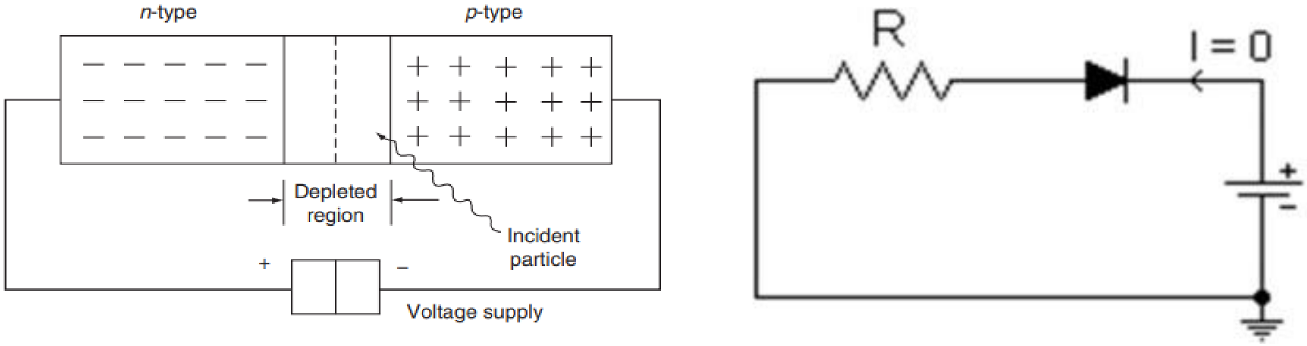
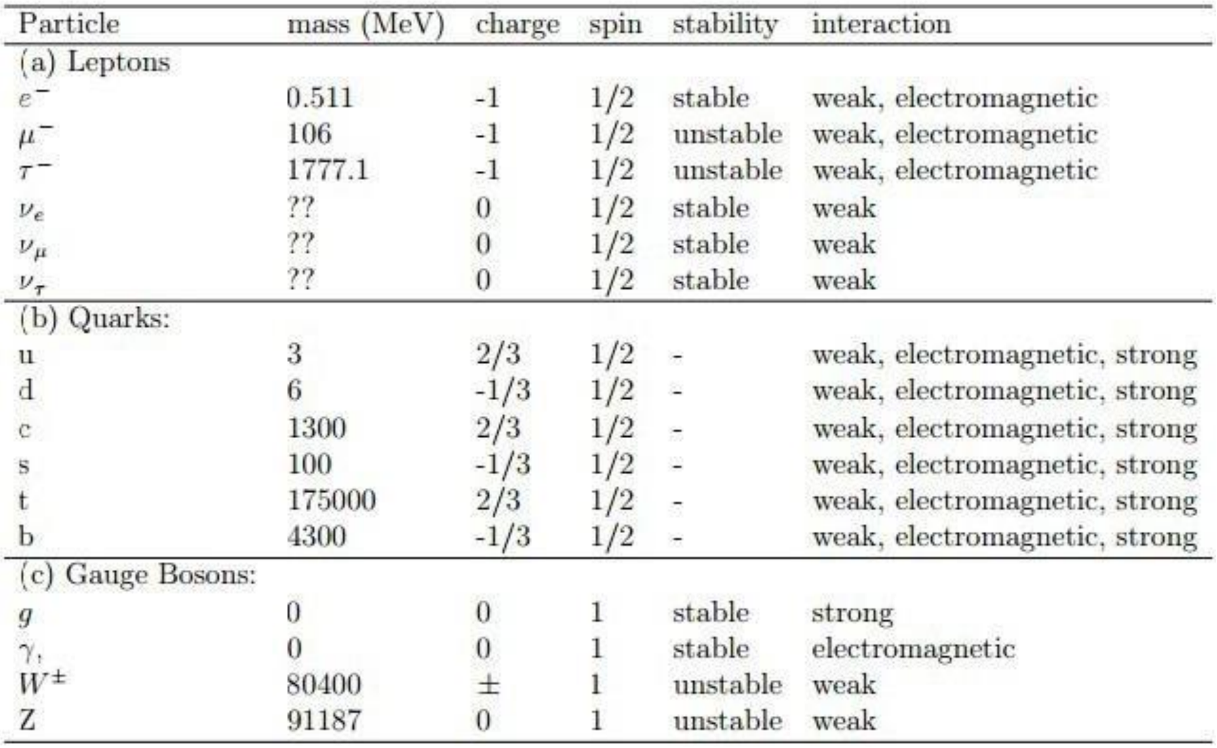


FIGURE : Solid-state n-p junction detector

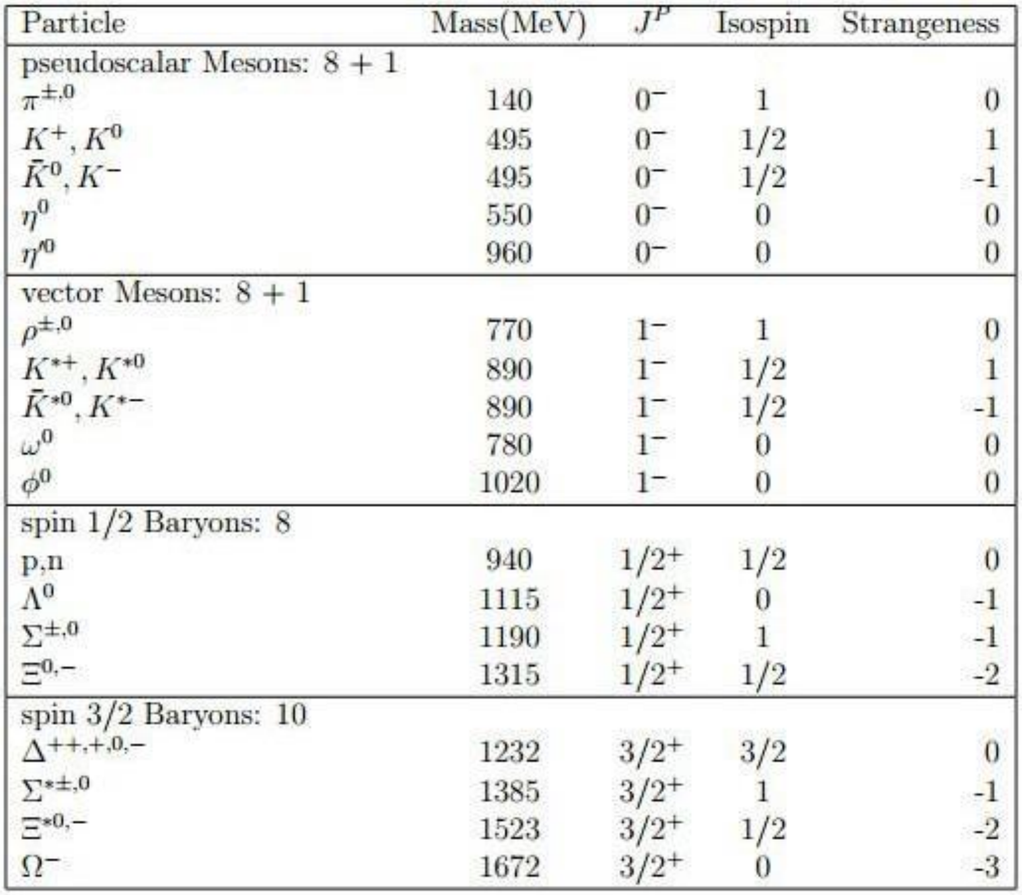
The important features of semiconductor detectors are their superior energy resolution due to a lower ionization potential and compact size.

Elementary Particles: A particle which does not have a sub structure or those microscopic elementary constituents out of which all matter in this universe is considered to be made of. All elementary particles are either bosons or fermions. These classes are distinguished by their quantum statistics: fermions obey Fermi–Dirac statistics and bosons obey Bose–Einstein statistics. Their spin is differentiated via the spin–statistics theorem. it is half-integer for fermions, and integer for bosons.

Classification of elementary particles:



Particle	mass (MeV)	charge	spin	stability	interaction
(a) Leptons					
e^-	0.511	-1	1/2	stable	weak, electromagnetic
μ^-	106	-1	1/2	unstable	weak, electromagnetic
τ^-	1777.1	-1	1/2	unstable	weak, electromagnetic
ν_e	??	0	1/2	stable	weak
ν_μ	??	0	1/2	stable	weak
ν_τ	??	0	1/2	stable	weak
(b) Quarks:					
u	3	2/3	1/2	-	weak, electromagnetic, strong
d	6	-1/3	1/2	-	weak, electromagnetic, strong
c	1300	2/3	1/2	-	weak, electromagnetic, strong
s	100	-1/3	1/2	-	weak, electromagnetic, strong
t	175000	2/3	1/2	-	weak, electromagnetic, strong
b	4300	-1/3	1/2	-	weak, electromagnetic, strong
(c) Gauge Bosons:					
g	0	0	1	stable	strong
γ	0	0	1	stable	electromagnetic
$W^\pm$	80400	±	1	unstable	weak
Z	91187	0	1	unstable	weak



Particle	Mass(MeV)	J^P	Isospin	Strangeness
pseudoscalar Mesons: 8 + 1				
$\pi^{\pm,0}$	140	0^-	1	0
K^+, K^0	495	0^-	1/2	1
$\bar{K}^0, K^-$	495	0^-	1/2	-1
η^0	550	0^-	0	0
η'^0	960	0^-	0	0
vector Mesons: 8 + 1				
$\rho^{\pm,0}$	770	1^-	1	0
K^{*+}, K^{*0}	890	1^-	1/2	1
$\bar{K}^{*0}, K^{*-}$	890	1^-	1/2	-1
ω^0	780	1^-	0	0
ϕ^0	1020	1^-	0	0
spin 1/2 Baryons: 8				
p,n	940	$1/2^+$	1/2	0
Λ^0	1115	$1/2^+$	0	-1
$\Sigma^{\pm,0}$	1190	$1/2^+$	1	-1
$\Xi^{0,-}$	1315	$1/2^+$	1/2	-2
spin 3/2 Baryons: 10				
$\Delta^{++,+,0,-}$	1232	$3/2^+$	3/2	0
$\Sigma^{*\pm,0}$	1385	$3/2^+$	1	-1
$\Xi^{*0,-}$	1523	$3/2^+$	1/2	-2
Ω^-	1672	$3/2^+$	0	-3

Table 4.1: Hadrons and their properties

HERE ARE SOME REFERENCES FOR AN INTRODUCTION TO NUCLEAR PHYSICS:

Textbooks:

1. "Nuclear Physics" by S. S. M. Wong
2. "Introduction to Nuclear Physics" by K. S. Krane
3. "Nuclear Physics: A Comprehensive Introduction" by J. M. Eisenberg and W. Greiner
4. "The Nuclear Physics Handbook" by C. W. Leroy and S. J. Rimjaem
5. "Nuclear Physics: Principles and Applications" by J. S. Lilley

Research Journals:

1. Nuclear Physics A
2. Nuclear Physics B
3. Physical Review C: Nuclear Physics
4. Journal of Nuclear Physics
5. European Physical Journal A: Hadrons and Nuclei

Online Resources:

1. National Nuclear Data Center (NNDC)
2. Nuclear Physics Group, University of Oxford
3. American Physical Society (APS) - Division of Nuclear Physics
4. HyperPhysics - Nuclear Physics
5. Nuclear Physics Laboratory, University of Washington

Historical Papers:

1. Ernest Rutherford, "The Scattering of α-Particles by Gas Molecules" (1911)
2. Niels Bohr, "On the Constitution of Atoms and Molecules" (1913)
3. Werner Heisenberg, "The Uncertainty Principle" (1927)
4. Enrico Fermi, "Tentative Theory of Nuclear Reactions" (1934)
5. Otto Hahn and Fritz Strassmann, "Discovery of Nuclear Fission" (1939)

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E-Notes

Subject: Zoology

(Study material for Undergraduate Students)

B.Sc IV Sem

COURSE CODE: DSCC5ZOOT4

Core Course Content: Gene Technology Immunology and Computational Biology

Unit III: Bioinformatics

Developed by: Smt. S. R. Deshpande

Bioinformatics

Definition: Bioinformatics studies the genetic make-up of all living organisms to answer complex biological questions through the development of new information technologies. It is multidisciplinary field, which combines information technology, computer science and biology. Information science has been applied to biology to produce the field called *Bioinformatics.*

Bioinformatics is a subdiscipline of biology and computer science concerned with the acquisition, storage, analysis, and dissemination of biological data, most often DNA and amino acid sequences. Bioinformatics uses computer programs for a variety of applications, including determining gene and protein functions, establishing evolutionary relationships, and predicting the three-dimensional shapes of proteins.

Goals of Bioinformatics:

To increase the understanding of various biological techniques/ processes like:

- Mapping & analysis of DNA, RNA & Protein.
- To study/ view/create 3D models of protein structures.
- To organizes data in a way that allows researchers to access existing information & to submit new entries as they are produced. E.g. Protein Database bank (PDB) for3D macromolecular structures.
- Developing methods to predict the structure and function of newly discovered DNA, RNA & Proteins and structural sequences. e.g., Sequence Analysis.
- Clustering protein sequences into families of related sequences and the development of protein models (Molecular Modeling).
- Aligning similar proteins and generate Phylogenetic trees to examine evolutionary relationships within the different organisms.
- To combine theory and practice to help solve research problems.
- Identification of mutation that led to disease.
- To define and develop new algorithms and statistics to assess relationships among large datasets.
- Analysis and interpretation of various types of data including nucleotide, amino acid sequences, EST, STS, Motif, RNA, Protein domains and Protein structures.
- The development and implementation of bio tools that enable efficient access and management of different types of genetic information.

Construction of databases:

Biological databases consist of long strings of nucleotides (DNA, RNA i.e. A T G C or U) as well as amino acids. Each sequence of nucleotides or amino acids represents a particular gene or protein (or section thereof), respectively. Sequences are represented in shorthand, using single letter designations. This decreases the space necessary to store information and increases processing speed for analysis.

While most biological databases contain nucleotide and protein sequence information, there are also databases, which include molecular pathways, protein structures, taxonomic information and the biochemical characteristics of organisms.

Types of Databases:

1. **Primary databases**: Primary databases store and make data available to the public, acting as repositories. In primary databases to provide layers of information to DNA or amino acid sequence data.

   For example: Genbank (NCBI), EMBL and DDBJ, Swissprot, Uniprot

2. **Secondary databases**: Secondary databases comprise data derived from analyzing entries in primary databases. It is database of secondary structure of protein motifs, regular expressions etc and are applied to the protein sequences rather than nucleotide sequences.
   For example: BIOGRID, STRING
3. **Tertiary databases:** includes tertiary protein structure which includes domains, folding units of proteins and atomic coordination.
   For example: PDB, CATH, SCOPE

Some abbreviations of Database centers:

1. **NCBI:** National Center of Biotechnology Information.
2. **EMBL**: European Molecular Biology Laboratory.
3. **DDBJ**: DNA Database Bank of Japan.
4. **BioGRID**: The Biological General Repository for Interaction Datasets.
5. **STRING:** Search Tool for the Retrieval of Interacting Genes/Proteins
6. **PDB:** Protein Database bank
7. **CATH:** class architecture topology homology
8. **SCOPE**: Structural classification of protein.
9. **INSDC:** International Nucleotide Database Centre.
10. **OMIM:** Online Mendelian Inheritance of Man.
11. World Wide Web, the Cancer Biomedical Informatics Grid (caBIG)

Applications of Bioinformatics:

- Bioinformatics is being used in following fields
- Molecular Medicine, Personalized Medicine, Preventive Medicine, Medical Informatics.
- Gene Manipulation Gene therapy.
- New Drug Discovery and Development. Like rational, structural, protein, cell etc based drug design and also Computer-Assisted Drug Design.
- Plant Genomics and Proteomics Crop Improvement.
- Identification of SNPs- Single Nucleotide Polymorphism: It is possible to predict the variation of genes for drug response due to SNPs. SNPs (pronounced "snips") as they are commonly called single nucleotide polymorphism. It can be used as a diagnostic tool to predict a person's drug response.
- Pharmacogenomics and Pharmacogenetics. RNA interference (RNAi) is one of the most exciting discoveries of the past decade in functional genomics.
- Microbial Genome Applications.
- **In Biotechnology field. Like**
    - PCR- Polymerase Chain Reaction.
    - rDNA - Recombinant DNA Technology.
    - DNA Microarray technology- DNA Chips, Protein Chips, Tissue Microarray.
    - Tissue Culture Technology.
    - Genetic Engineering.
    - Transgenic Plant and GM (Genetically Modified) Crop.
    - Cloning Technology.
    - DNA fingerprinting.

Study of Drug / Antibiotic Resistance.

- Protein Drug Interaction.
- Target based Drug Development.
- Metabolic Pathway Analysis.

Evolutionary Studies.

- Phylogenetic Homology Analysis.
- Phylogenomic and Evolutionary Genomics.
- Evolutionary Study of Different Species.
- Lateral Gene Transfer and Mutational Analysis.

- **Insect Resistance:** The identification of genes controlling important metabolic pathways such as for insect resistance, isolation of genes of various types, phytochemical analysis, study of natural product, secondary metabolites, determination of directional pathways of evolution and location of useful genes from exotic sources, decision making on biodiversity conservation.
- **Improve Nutritional Quality:** Bioinformatics and plant genomics illustrates the identification of homologous genes and traits, and explores breeding opportunities based on comparative genetics. Plant's genomics research will lead to new and innovative ways to achieve such trait improvement by the use of bioinformatics.
- Forest Informatics and Development of Drought resistance varieties.
- Veterinary Science.
- Waste cleanup and study of alternative energy sources.

Sequence Analysis:

Margaret Dayhoff (1972, 1978) and her collaborators at the *National Biomedical Research Foundation (NBRF), Washington, DC,* were the first to assemble databases of these sequences into a protein sequence atlas in the 1960.
In bioinformatics, sequence analysis is the process of subjecting a DNA, RNA or peptide sequence to any of a wide range of analytical methods to understand its features, function, structure, or evolution.

It includes

- **Sequencing:** DNA sequencing is the process of determining the precise order of nucleotides or order of the bases. Protein sequencing is a technique to determine the amino acid sequence of protein, as well as conformation the protein adopts and the extent to which it is complexed with non-peptide molecules.

- **Sequencing assembly:** Refers to the reconstruction of DNA sequence by aligning & merging smaller fragments of DNA. It is integral part of modern DNA sequencing.
  a. Cutting DNA into small pieces b. reading small fragments. c. reconstituting original DNA by merging the information on various fragment.

- **Sequence Alignment:** It is a way of arranging the sequences of DNA, RNA and protein to identify similarity that may be a consequence of functional, structural or evolutionary relationship between the sequences. It involves the identification of the correct location of deletions and insertions that have occurred either in either of two lineages since the divergence from a common ancestor.

- **Searching databases:** To know the query sequence by entering in the databases.

Sequence Alignments:
Sequence alignment is the procedure of comparing two (pair-wise alignment) or more (Multiple sequence alignment) sequences by searching for a series of individual characters or character patterns that are in the same order in the sequences. Two sequences are aligned by writing them across a page in two rows. Identical or similar characters are placed in the same column, and nonidentical characters can either be placed in the same column as a mismatch or opposite a gap in the other sequence. Sequence Alignments can be used to detect homology between two polypeptide chains. Figuring out sequence alignments can help develop evolutionary origins and trace back the function, structure, and mechanism of a genome. Repeated motifs can be detected by aligning a sequence with itself.

Types of Sequence Alignments:

1. **Local Alignments:** In local alignment, stretches of sequence with the highest density of matches are aligned, thus generating one or more islands of matches or subalignments in the aligned sequences. Local alignments are more suitable for aligning sequences that are similar along some of their lengths but dissimilar in others, sequences that differ in length, or sequences that share a conserved region or domain.
2. **Global sequence alignment:** In global alignment, an attempt is made to align the entire sequence, using as many characters as possible, up to both ends of each sequence. Sequences that are quite similar and approximately the same length are suitable candidates for global alignment.
   Seq 1 - TAGC-GC-GT 2) *Seq 2* -TA-CA-CAGT.

SIGNIFICANCE OF SEQUENCE ALIGNMENT

- Sequence alignment is useful for discovering functional, structural, and evolutionary information in biological sequences.
- It is important to obtain the best possible or so-called “optimal” alignment to discover this information.
- Sequences that are very much alike, or “similar” in the parlance of sequence analysis, probably have the same function, be it a regulatory role in the case of similar DNA molecules, or a similar biochemical function and three-dimensional structure in the case of proteins.
- Additionally, if two sequences from different organisms are similar, there may have been a common ancestor sequence, and the sequences are then defined as being homologous.
- The alignment indicates the changes that could have occurred between the two homologous sequences and a common ancestor sequence during evolution.

Types of Sequence Alignments on the basis of number of comparing sequencing strand, it is of two types.

1. **Pair wise alignment:** It compares only two sequences at a time. It consists of pairwise alignment consists of series of paired bases, one base from each sequence. There are three types of pairs.
    - A. *Matches*= same nucleotides appear in both sequences.
    - B. *Mismatches*=Different nucleotides are found in the two sequences.
    - C. *Gaps*=a base in one sequence and null base in the other.

2. **Multiple sequence Alignment (MSA):** a multiple alignment are three or more protein sequences, the highly conserved residues that define structural and functional domains in protein families can be identified. New members of such families can then be found by searching sequence databases for other sequences with these same domains. Alignment of DNA sequences can assist in finding conserved regulatory patterns in DNA sequences.

BLAST:

BLAST stands for **Basic Alignment Search Tool**. Blast is a program which uses specific scoring matrices for performing sequence similarity searches against a variety of sequence databases, to give us high scoring ungapped segments among related sequences.

BLAST is an algorithm for comparing primary biological sequence information, such as the amino-acid sequence. The BLAST algorithm and program were designed by *Stephen Altschul, Warren Gish, Webb Miller, Eugene Myers, and David J. Lipman at.al* the **National Institutes of Health of USA.**

Characteristics of BLAST

- BLAST algorithm is fast, accurate and web accessible.
- Enables researcher to compare a query sequence with a library or database sequence.
- Discovering new genes or proteins
- Exploring protein structure and function.
- It is relatively faster than any other search tools.
- Provides us with ability to perform analysis by different types of programs.
- To find high scoring ungapped segments among related sequences.
- Investigating expressed sequence tags (ESTS)
- BLAST uses a heuristic approach it is not guaranteed to be the optimal answer, but is close to it.

BLAST is available at https://blast.ncbi.nlm.nih.gov

How BLAST works:

BLAST first searches for short regions of a given length (W) called "words" (or substrings) that score at least "T" when compared to the query sequence that align with sequences in the databases (Target sequences) using substation matrix.

For every pair of sequences (query & Target) that have a word or words in common, BLAST extends the alignment in both directions to find alignments that score greater (are more similar) that certain score threshold(S). these alignments are called *high scoring pairs or HSPs.*

BLAST Input-Output

Input:

- Query sequence Q (11 nucleotide bases is one word for DNA & 3 amino acid is one word for protein. L-W+1. L=Length of sequence & W=Words)
- Database sequence DB
- Minimal score S
- Input sequences in FASTA or Genbank format

Output:

- Sequences from DB (seq) such that Q and seq have score >S.
- Can be delivered in variety of formats. These formats include HTML, plain text & XML formatting.

E- value (Expectation Value)

The expect value (E) is a parameter that describes the number of hits one can "expect" to see by chance when searching a database of particular size.

Types of BLAST:

BLASTn – Nucleotide-nucleotide

Blastp – Protein-protein

Blastpgp-Position specific Iterative BLAST

Blastx- nucleotide 6-frame translation protein

Of these programs, BLASTn & BLASTpare the most commonly used because they use direct comparisons, and do not require translations.

FASTA

FASTA stands for fast-all" or "FastA". It was the first database similarity search tool developed, preceding the development of BLAST.FASTA package was 1st described by *Lipman & Pearson* in 1985.

It derived from dot-plot compute the best diagonals from all frames of alignments.

Features of FASTA

- It finds out patches of sequence Similarity between the query & database.
- FASTA maintains the GAPS well.
- Identification of species.
- Establishing phylogeny.
- DNA mapping.
- Understanding biochemical functions of protein.
- Studying evolution of species.
- Identification of mutations.
- Calculating molecular weight.
- Knowing amino acid composition.

How FASTA works?

- Similarity of matching words (6 nucleotide bases – one word in DNA & 3amino acid = one word in protein sequence.
- Does not require identical words.
- A sequence in FASTA format begins with a single-line description, followed by lines of sequence data. The description line is distinguished from the sequence data by a greater-than (">") symbol in the first column.

- The word following the ">" symbol is the identifier of the sequence, and the rest of the line is the description (both are optional). There should be no space between the ">" and the first letter of the identifier.
- It is recommended that all lines of text be shorter than 80 characters. The sequence ends if another line starting with a ">" appears; this indicates the start of another sequence.
- A sequence in FASTA format is represented as a series of lines, each of which should be no longer than 120 characters and usually do not exceed 80 characters.

CLUSTALW

CLUSTALW is a widely used software tool for performing **multiple sequence alignment (MSA)** of biological sequences, such as DNA, RNA, or protein sequences. It aims to align multiple sequences in such a way that the homologous positions across the sequences are matched, helping researchers identify conserved regions and functional motifs.

The key details and steps involved in the CLUSTALW algorithm for multiple sequence alignment:

1. **Input Sequences**: CLUSTALW takes as input a set of biological sequences in FASTA format or other common sequence file formats. These sequences are usually related in terms of function or evolutionary history.
2. **Pairwise Sequence Alignment**: CLUSTALW begins by performing pairwise sequence alignments using dynamic programming algorithms (like **Needleman-Wunsch or Smith-Waterman)** to align every pair of sequences. This step generates a similarity score matrix that measures the similarity between each pair of sequences.
3. **Guide Tree Construction**: The next step involves constructing a guide tree or a phylogenetic tree.
4. **Progressive Alignment**: CLUSTALW performs progressive multiple sequence alignment based on the guide tree. It starts by aligning the most closely related sequences according to the tree and gradually adds more sequences into the alignment, extending it progressively. This process involves aligning sequences based on the **similarity scores** obtained from the pairwise alignments and the guide tree.
5. **Profile Alignment**: As the alignment is built progressively, a profile is created for the aligned sequences. The profile represents a position-specific score matrix that accounts for the amino acid or nucleotide distribution at each aligned position.
6. **Final Alignment**: The iterative process continues until convergence or a predefined number of iterations is reached. The resulting alignment is the final multiple sequence alignment.
7. **Output**: CLUSTALW generates an output file that contains the aligned sequences in a format that displays the aligned positions, gaps, and consensus sequences. The alignment file can be further analysed to identify conserved motifs, evolutionary relationships, and functional insights.

- **References:**

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Dept. of Mathematics

Course Title: Algebra-I and Calculus-I (DSC)

Course Code: 126BSC01MATDSC91T

Class: B.Sc I semester

Matrix

Introduction

Matrix is a rectangular array of numbers, symbols, points, or characters each belonging to a specific row and column. A matrix is identified by its order which is given in the form of rows × and columns. The numbers, symbols, points, or characters present inside a matrix are called the elements of a matrix. The location of each element is given by the row and column it belongs to.

Matrices are important for students of class 12 and are also of great importance in engineering mathematics. We will learn about the types of matrices, the transpose of matrices, the rank of matrices.

What are Matrices?

Matrices are rectangular arrays of numbers, symbols, or characters where all of these elements are arranged in each row and column. An array is a collection of items arranged at different locations.

Matrix in Mathematics $\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$

Matrix Definition:

A rectangular array of numbers, symbols, or characters is called a Matrix.
Matrices are identified by their order. The order of the matrices is given in the form of a number of rows × number of columns. A matrix is represented as

[P]m×n where P is the matrix, m is the number of rows and n is the number of columns. Matrices in mathematics are useful in solving numerous problems of linear equations and many more.

Order of Matrix

Order of a Matrix tells about the number of rows and columns present in a matrix. Order of a matrix is represented as the number of rows times the number of columns. Let's say if a matrix has 4 rows and 5 columns then the order of the matrix will be 4×5. Always remember that the first number in the order signifies the number of rows present in the matrix and the second number signifies the number of columns in the matrix.

Matrices Examples

Examples of matrices are mentioned below:

Example: $\begin{bmatrix} 1 & 2 & 3 \\ 6 & 2 & -2 \\ 4 & 5 & 3 \end{bmatrix}_{3X3}$ $\begin{bmatrix} 1 & 3 \\ 2 & 7 \end{bmatrix}_{2X2}$

Operation on Matrices

Matrices undergo various mathematical operations such as addition, subtraction, scalar multiplication, and multiplication. These operations are performed between the elements of two matrices to give an equivalent matrix that contains the elements which are obtained as a result of the operation between elements of two matrices. Let's learn the operation of matrices.

Addition of Matrices

In addition of matrices, the elements of two matrices are added to yield a matrix that contains elements obtained as the sum of two matrices. The addition of matrices is performed between two matrices of the same order.

Example: Find the sum of $\begin{bmatrix} 1 & 3 & 4 \\ 2 & -1 & 6 \end{bmatrix}$ **and** $\begin{bmatrix} 1 & -2 & 5 \\ 2 & 4 & 6 \end{bmatrix}$

Solution:

Here, we have $A = \begin{bmatrix} 1 & 3 & 4 \\ 2 & -1 & 6 \end{bmatrix}$ *and* $B = \begin{bmatrix} 1 & -2 & 5 \\ 2 & 4 & 6 \end{bmatrix}$

$$A + B = \begin{bmatrix} 1 & 3 & 4 \\ 2 & -1 & 6 \end{bmatrix} + \begin{bmatrix} 1 & -2 & 5 \\ 2 & 4 & 6 \end{bmatrix}$$

$$\Rightarrow A + B = \begin{bmatrix} 1+1 & 3-2 & 4+5 \\ 2+2 & -1+4 & 6+6 \end{bmatrix}$$

$$\Rightarrow A + B = \begin{bmatrix} 2 & 1 & 11 \\ 4 & 3 & 12 \end{bmatrix}$$

Subtraction of Matrices

Subtraction of Matrices is the difference between the elements of two matrices of the same order to give an equivalent matrix of the same order whose elements are equal to the difference of elements of two matrices. The subtraction of two matrices can be represented in terms of the addition of two matrices. Let’s say we have to subtract matrix B from matrix A then we can write A – B. We can also rewrite it as A + (-B). Let’s solve an example

Example: Subtract $\begin{bmatrix} 2 & 5 & 3 \\ 5 & 3 & 7 \\ 2 & -5 & 4 \end{bmatrix}$ **from** $\begin{bmatrix} 1 & 8 & 6 \\ 5 & 3 & 4 \\ 5 & 7 & 6 \end{bmatrix}$

Let us assume $A = \begin{bmatrix} 2 & 5 & 3 \\ 5 & 3 & 7 \\ 2 & -5 & 4 \end{bmatrix}$ *and* $B = \begin{bmatrix} 1 & 8 & 6 \\ 5 & 3 & 4 \\ 5 & 7 & 6 \end{bmatrix}$

$$A - B = \begin{bmatrix} 2 & 5 & 3 \\ 5 & 3 & 7 \\ 2 & -5 & 4 \end{bmatrix} - \begin{bmatrix} 1 & 8 & 6 \\ 5 & 3 & 4 \\ 5 & 7 & 6 \end{bmatrix}$$

$$\Rightarrow A - B = \begin{bmatrix} 2-1 & 5-8 & 3-6 \\ 5-5 & 3-3 & 7-4 \\ 2-5 & -5-7 & 4-6 \end{bmatrix}$$

$$\Rightarrow A - B = \begin{bmatrix} 1 & -3 & -3 \\ 0 & 0 & 3 \\ -3 & -12 & -2 \end{bmatrix}$$

Scalar Multiplication of Matrices

Scalar Multiplication of matrices refers to the multiplication of each term of a matrix with a scalar term. If a scalar let's 'k' is multiplied by a matrix then the equivalent matrix will contain elements equal to the product of the scalar and the element of the original matrix.

Let's see an example:

Example: Multiply 3 with $\begin{bmatrix} 2 & 6 \\ 8 & 5 \end{bmatrix}$

$3[A] = \begin{bmatrix} 6 & 18 \\ 24 & 15 \end{bmatrix}$

Multiplication of Matrices

In the multiplication of matrices, two matrices are multiplied to yield a single equivalent matrix. The multiplication is performed in the manner that the elements of the row of the first matrix multiply with the elements of the columns of the second matrix and the product of elements are added to yield a single element of the equivalent matrix. If a matrix $[A]_{i\times j}$ is multiplied with matrix $[B]_{j\times k}$ then the product is given as $[AB]_{i\times k}$.

Let's see an example.

Example: Find the product of $\begin{bmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{3} & \mathbf{4} \end{bmatrix}$ **and** $\begin{bmatrix} \mathbf{2} & \mathbf{-1} \\ \mathbf{3} & \mathbf{6} \end{bmatrix}$

Solution:

Let A = $\begin{bmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{3} & \mathbf{4} \end{bmatrix}$ ***and B =*** $\begin{bmatrix} \mathbf{2} & \mathbf{-1} \\ \mathbf{3} & \mathbf{6} \end{bmatrix}$

$$\Rightarrow AB = \begin{bmatrix} \mathbf{2+0} & \mathbf{-1+0} \\ \mathbf{6+12} & \mathbf{-3+24} \end{bmatrix}$$

$$\Rightarrow AB = \begin{bmatrix} \mathbf{2} & \mathbf{-1} \\ \mathbf{18} & \mathbf{21} \end{bmatrix}$$

Properties of Matrix Addition and Multiplication

Properties followed by Multiplication and Addition of Matrices is listed below:

- A + B = B + A (Commutative)
- (A + B) + C = A + (B + C) (Associative)
- AB ≠ BA (Not Commutative)
- (AB) C = A (BC) (Associative)
- A (B+C) = AB + AC (Distributive)

Transpose of Matrix

Transpose of Matrix is basically the rearrangement of row elements in column and column elements in a row to yield an equivalent matrix. A matrix in which the elements of the row of the original matrix are arranged in columns or vice versa is called Transpose Matrix. The transpose matrix is represented as A^T.

Let's see an example:

Example: Find the transpose of the matrix A= $\begin{bmatrix} \mathbf{1} & \mathbf{-2} & \mathbf{5} \\ \mathbf{2} & \mathbf{4} & \mathbf{6} \end{bmatrix}$**.**

Solution:

$Let\ A = \begin{bmatrix} 1 & -2 & 5 \\ 2 & 4 & 6 \end{bmatrix}$

$$\Rightarrow A^T = \begin{bmatrix} 1 & 2 \\ -2 & 4 \\ 5 & 6 \end{bmatrix}$$

Properties of the Transpose of a Matrix

Properties of the transpose of a matrix are mentioned below:

- $(A^T)^T$= A
- $(A + B)^T = A^T + B^T$
- $(AB)^T = B^T A^T$

Trace of Matrix

Trace of a Matrix is the sum of the principal diagonal elements of a square matrix. Trace of a matrix is only found in the case of a square matrix because diagonal elements exist only in square matrices.
Let's see an example.

Example: Find the trace of the matrix A=$\begin{bmatrix} \mathbf{2} & \mathbf{5} & \mathbf{3} \\ \mathbf{5} & \mathbf{3} & \mathbf{7} \\ \mathbf{2} & \mathbf{-5} & \mathbf{4} \end{bmatrix}$

Solution:

Let us assume A = $\begin{bmatrix} 2 & 5 & 3 \\ 5 & 3 & 7 \\ 2 & -5 & 4 \end{bmatrix}$

Trace(A) = 2+ 3 + 4 = 9

Types of Matrices

Based on the number of rows and columns present and the special characteristics shown, matrices are classified into various types.

- **Row Matrix:** A Matrix in which there is only one row and no column is called Row Matrix.

- **Column Matrix:** A Matrix in which there is only one column and now row is called a Column Matrix.

- **Horizontal Matrix:** A Matrix in which the number of rows is less than the number of columns is called a Horizontal Matrix.

- **Vertical Matrix:** A Matrix in which the number of columns is less than the number of rows is called a Vertical Matrix.

- **Rectangular Matrix:** A Matrix in which the number of rows and columns are unequal is called a Rectangular Matrix.

- **Square Matrix:** A matrix in which the number of rows and columns are the same is called a Square Matrix.

- **Diagonal Matrix:** A square matrix in which the non-diagonal elements are zero is called a Diagonal Matrix.

- **Zero or Null Matrix:** A matrix whose all elements are zero is called a Zero Matrix. A zero matrix is also called as Null Matrix.

- **Unit or Identity Matrix:** A diagonal matrix whose all diagonal elements are 1 is called a Unit Matrix. A unit matrix is also called an Identity matrix. An identity matrix is represented by I.

- **Symmetric matrix:** A square matrix is said to be symmetric if the transpose of the original matrix is equal to its original matrix. i.e. $(A)^T = A$

  Skew-symmetric Matrix: A skew-symmetric (or antisymmetric or antimetric[1]) matrix is a square matrix whose transpose equals its negative i.e. $(A)^T = -A$

- **Involutory Matrix:** A matrix is said to be Involutory if A2 = I.

- **Upper Triangular Matrix:** A square matrix in which all the elements below the diagonal are zero is known as the upper triangular matrix

- **Lower Triangular Matrix:** A square matrix in which all the elements above the diagonal are zero is known as the lower triangular matrix
- **Singular Matrix:** A square matrix is said to be a singular matrix if its determinant is zero i.e. |A|=0
- **Nonsingular Matrix:** A square matrix is said to be a non-singular matrix if its determinant is non-zero.

Properties of Symmetric Matrix

- Addition and difference of two symmetric matrices results in symmetric matrix.
- If A and B are two symmetric matrices and they follow the commutative property, i.e. AB =BA, then the product of A and B is symmetric.
- If matrix A is symmetric then A^n is also symmetric, where n is an integer.
- If A is a symmetric matrix then A^{-1} is also symmetric.

Let us take example.

$$B = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 4 & 6 \\ 3 & 6 & 7 \end{bmatrix}$$

If we take the transpose of this matrix, we will get:

$$B' = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 4 & 6 \\ 3 & 6 & 7 \end{bmatrix}$$

We see that B = B'. Whenever this happens for any matrix, that is whenever transpose of a matrix is equal to it, the matrix is known as a **symmetric matrix**. But how can we find whether a matrix is symmetric or not without finding its transpose? We know that:

If $A = [a_{ij}]_{mXn}$ $then\ A' = [a_{ij}]_{nXm}$ (for all the values of i and j)
So, if for a matrix A, $a_{ij} = a_{ji}$ (for all the values of i and j) and m = n, then its transpose is equal to itself. A symmetric matrix will hence always be square.

Skew Symmetric Matrix

A matrix can be skew symmetric only if it is square. If the transpose of a matrix is equal to the negative of itself, the matrix is said to be **skew symmetric**. This means that for a matrix to be skew symmetric,

A'=-A Also, for the matrix, $a_{ji} = -a_{ij}$(for all the values of i and j). The diagonal elements of a skew symmetric matrix are equal to zero. This can be proved in following way:

The diagonal elements are characterized by the general formula,

a_{ij} , where i = j

If i = j, then $a_{ij} = a_{ii} = a_{jj}$

If A is skew symmetric, then

$a_{ji} = – a_{ji}$

$\Rightarrow a_{ii} = – a_{ii}$

⇒ $2.a_{ii} = 0$

⇒ $a_{ii} = 0$

So, $a_{ij} = 0$, when i = j (for all the values of i and j)

Some examples of skew symmetric matrices are:

$$A = \begin{bmatrix} 0 & -5 \\ 5 & 0 \end{bmatrix} \qquad B = \begin{bmatrix} 0 & 2 & 4 \\ -2 & 0 & 5 \\ -4 & -5 & 0 \end{bmatrix}$$

Properties of Skew Symmetric Matrix

- When we add two skew-symmetric matrices then the resultant matrix is also skew-symmetric.
- Scalar product of skew-symmetric matrix is also a skew-symmetric matrix.
- The diagonal of skew symmetric matrix consists of zero elements and therefore the sum of elements in the main diagonals is equal to zero.
- When identity matrix is added to skew symmetric matrix then the resultant matrix is invertible.
- The determinant of skew symmetric matrix is non-negative

Elementary Transformation of a matrix:

The following operation on a matrix are called elementary operations (transformations)

1. The interchange of any two rows (or columns)
2. The multiplicationof the elements of any row (or column) by any nonzero number
3. The addition to the elements of any row (or column) the corresponding elements of any other row (or column) multiplied by any number

Echelon Form of matrix : A matrix A is said to be in echelon form if

(i) every row of A which has all its elements 0, occurs below row, which has a non-zero elements

(ii) the first non-zero element in each non –zero row is 1.

(iii) The number of zeros before the first non zero elements in a row is less than the number of such zeros in the next now.

[A row of a matrix is said to be a zero row if all its elements are zero]

Note: Rank of a matrix does not change by application of any elementary operations

For example $A = \begin{bmatrix} 1 & 2 & 5 \\ 0 & 5 & 8 \\ 0 & 0 & 11 \end{bmatrix} \quad B = \begin{bmatrix} 1 & 6 & 5 & 4 \\ 0 & 0 & 3 & 7 \\ 0 & 0 & 0 & 8 \end{bmatrix}$

The number of non-zero rows in the echelon form of a matrix is defined as its RANK.

Rank of a matrix:

A matrix A is said to have rank r if

i) there exists at least one minor of order r of the matrix A which does not vanish.

ii) all minors of order r+1 must vanish.

Find the rank of matrix A by using the row echelon form where $\boldsymbol{A} = \begin{bmatrix} \mathbf{1} & \mathbf{2} & \mathbf{3} \\ \mathbf{2} & \mathbf{1} & \mathbf{4} \\ \mathbf{3} & \mathbf{0} & \mathbf{5} \end{bmatrix}$

Solution:

Given, $\boldsymbol{A} = \begin{bmatrix} \mathbf{1} & \mathbf{2} & \mathbf{3} \\ \mathbf{2} & \mathbf{1} & \mathbf{4} \\ \mathbf{3} & \mathbf{0} & \mathbf{5} \end{bmatrix}$

Now, we apply elementary transformations. $R_2 \rightarrow R_2 - 2R_1$ $R_3 \rightarrow R_3 - 3R_1$

We get $\begin{bmatrix} 1 & 2 & 3 \\ 0 & -3 & -2 \\ 0 & -6 & -4 \end{bmatrix}$

$R_3 \rightarrow R_3 - 2R_2$ $\begin{bmatrix} 1 & 2 & 3 \\ 0 & -3 & -2 \\ 0 & 0 & 0 \end{bmatrix}$

The above matrix is in row echelon form.

Number of non-zero rows = 2

Hence, the rank of matrix A = 2

SOLUTION OF A SYSTEM OF LINEAR EQUATIONS

Consider the system of equations

$$a_1x + b_1y + c_1z = d_1, \quad a_2x + b_2y + c_2z = d_2 , \quad a_3x + b_3y + c_3z = d_2$$

(3 equations in 3 unknowns)

In matrix notation, these equations can be written as

$$\begin{bmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \end{bmatrix}$$

or AX =B

Where A=$\begin{bmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{bmatrix}$ is called the co-efficient matrix , X =$\begin{bmatrix} x \\ y \\ z \end{bmatrix}$ is the column matrix of unknowns,

B=$\begin{bmatrix} d_1 \\ d_2 \\ d_3 \end{bmatrix}$ is the column matrix of constants.

If $d_1 = d_2 = d_3 = 0$ then B = 0 and the matrix equation AX =B reduces to AX =0, Such a system of equations is called a system of homogeneous linear equations. If at least one of d_1, d_2, d_3 is non-zero, then B ≠ 0. Such a system of equations is called a system of non-homogeneous linear equations.

The matrix equation AX =B need not always have a solution. It may have no solution or a unique solution or an infinite number of solutions.

A system of equations having no solution is called an inconsistent system of equation. A system of equations having one or more solution is called a consistent system of equations.

For a system of non-homogeneous linear equations AX =B

i) if $\rho[A: B] \neq \rho[A]$ the system is inconsistent.

ii) if $\rho[A: B] = \rho[A] <$ number of unknowns, the system has an infinite number of solutions.

iii) if $\rho[A] = \rho[A] =$ number of unknowns, the system has a unique solution.

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E-notes

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INTRODUCTION

- The concept of non-expansive mappings in Banach spaces has a rich history that is closely tied to the study of fixed-point theory, optimization, and the geometry of Banach spaces. Here is an overview of the history and development of non-expansive mappings:
- In 2008, Suzuki introduced the concept of generalized nonexpansive mappings which is a condition on mappings called condition (C).
- **Early Developments**
  1. Fixed-Point Theorems in Banach Spaces (1920s-1930s): The study of non-expansive mappings in Banach spaces began with the foundational work on fixed-point theorems. The most famous result from this period is the Banach fixed-point theorem (also known as the Contraction Mapping Theorem), which applies to contraction mappings (mappings that strictly reduce distances between points). Although this theorem is not about non-expansive mappings per se (which do not necessarily reduce distances), it laid the groundwork for studying mappings in Banach spaces and their fixed points.
  2. Early Examples of Non-Expansive Mappings (1930s-1940s): The idea of non-expansive mappings, defined as mappings that do not increase the distance between any two points, arose naturally in various mathematical contexts. For example, in the context of iterative methods for solving equations, certain mappings naturally appeared as non-expansive. The formal study of non-expansive mappings, however, started to gain momentum only in the mid-20th century.
- **Applications and Further Developments**

Development of Iterative Methods (1970s-1980s): During this period, the study of iterative methods for approximating fixed points of non-expansive mappings became a major area of research. Researchers developed various algorithms, such as the krasnosel k ii-Mann iteration, for finding fixed points of non-expansive mappings in Banach spaces. These methods are widely used in numerical analysis and optimization, particularly in contexts where direct computation of fixed points is challenging.

Geometry of Banach Spaces and Non-Expansive Mappings (1980s-1990s): The geometric properties of Banach spaces, such as convexity, uniform convexity, and smoothness, were further explored to understand their implications for non-expansive mappings. The theory of asymptotically non-expansive mappings also emerged during this time, expanding the scope of fixed-point theory to include mappings that are not strictly non-expansive but still preserve certain distance properties asymptotically.

Non-Expansive Mappings in Metric Fixed-Point Theory (2000s-Present): The study of non-expansive mappings continues to be a dynamic area of research. Advances in metric fixed-point theory, often motivated by problems in optimization and algorithmic game theory, have further generalized the results for non-expansive mappings beyond the setting of Banach spaces to more general metric spaces. This includes studies in hyperbolic spaces and CAT(0) spaces, where the geometric conditions differ significantly from those in Banach spaces but still allow for meaningful results about non-expansive mappings.

❖ Contemporary Research

Modern Applications and Algorithmic Approaches: Non-expansive mappings are now a cornerstone in various applications, from optimization and machine learning to signal processing and image reconstruction. The focus of contemporary research is often on developing efficient algorithms for high-dimensional problems where non-expansive mappings naturally arise, such as in compressed sensing and deep learning. Moreover, stochastic variants of non-expansive mappings are increasingly being studied, broadening the applicability of these concepts in probabilistic and random environments.

❖ Summary

The history of non-expansive mappings in Banach spaces is marked by significant theoretical developments that have enhanced our understanding of fixed-point thory, the geometry of Banach spaces, and their applications. From the early foundational results of the 1960s to contemporary studies in metric spaces and algorithms, non-expansive mappings continue to be a central object of study in mathematics and its applications.

CHAPTER-1

BASIC TERMINOLGIES

Definition1.11 :NORM LINEAR FUNCTION: Let X be a vector space over k=ℝ or ₵ Suppose $\|\cdot\|: X \to \mathbb{R}$ is a map satisfying the following three conditions:

- $\| x \| \geq 0 \, for\ all\ x \in X,$
- $\| x \| = 0 \, iff \ x = 0 \, for\ all\ x \in X,$
- $\| \alpha x \| = |\alpha| \, \| x \| \ \ for\ every\ \alpha \in k\ and\ x \in X,$
- $\| x + y \| \leq \| x \| + \| y \|$ for every $x, y \in X$. [Triangle inequality]

Then $\|\cdot\|$ is called a norm on X and $(X, \|\cdot\|)$ is called a normed space over k.

Example: Euclidean Space ($\mathbb{R}^n$)

$\|\cdot\|: \mathbb{R}^n \to \mathbb{R}$ is a norm linear space difined by ,

$$\| x \|_2 = \left[\sum_{i=1}^{n} x_i^2\right]^{\frac{1}{2}} Where\ x = (x_1, x_2\ , x_3 \dots\dots..x_n)$$

$$for\ all\ x_i \in \mathbb{R}\ \forall\ 1 \leq i \leq n$$

Definition1.12 Banach space : A norm linear vector space (X, $\|\cdot\|$) is said be a Banach space if ,It is complete space .[Every cuachy sequence in X is convergent in X]

Example: $\|\cdot\|: \mathbb{R}^n \to \mathbb{R}$ is a norm linear space difined by,

$$\| x \|_2 = \left[\sum_{i=1}^{n} x_i^2\right]^{1/2}$$

Where $x = (x_1\ x_2, x_3, , \dots\dots..x_n)$ for all $x_i \in \mathbb{R}$ for all i

Definition1.13 **Uniform Banach space** : A banach space X is called uniformly convex if for each $\varepsilon \in (0,2]$ there is a $\delta > 0$ such that for $x, y \in X$,

$$\|x\| \leq 1, \quad \|y\| \leq 1,$$

$$\|x-y\| > \varepsilon$$

$$\text{Then} \quad \|\tfrac{x+y}{2}\| \leq \delta$$

Example: l^2 =$\{x = (x_n) | \sum_{n=1}^{\infty} |x_n|^2 < \infty\}$ norm defined by

$$\|x\| = \left(\sum_{n=1}^{\infty} |x_n|^2\right)^{\frac{1}{2}}$$

and ,$\|x\|_{\infty} = sup_n \; |x_n| \; for \; x = (x_n) \in l^{\infty}$ which is not satisfied

Definition1.14 **Opial property of Banach space :**A Banach space X is said to satisfy the Opial property , if for each sequence $\{x_n\} \; in \; X$, converging weakly to $x \in X$, we have

$\limsup\limits_{n\to\infty} \|\mathbf{x_n} - \mathbf{x}\|$ <$\limsup\limits_{n\to\infty} \|\mathbf{x_n} - \mathbf{y}\|$, for all $y \in X$ such that $y \neq x$.

Example: l^p =$\{x = (x_n) | \sum_{n=1}^{\infty} |x_n|^p < \infty\}$,$(1 < p < \infty)$ with norm defined by

$$\|x\| = \left(\sum_{n=1}^{\infty} |x_n|^p\right)^{\frac{1}{p}}$$

Definition1.15 **Fixed point of a mapping T** : Let Y be a nonempty subset of a Banach space X and a point **p** is called fixed point of a mapping $T : Y \to Y$ if $T(p) = p$, and $F(T)$ represents the set of all fixed points of mapping T.

Example: $T : \mathbb{R}^n \rightarrow \mathbb{R}^n$ defined by $T(x) = \frac{1}{2}x$,here $x = 0$ is fixed point of T

Definition1.16 **Contraction mapping**: Let Y be a nonempty subset of a Banach space X. A mapping $T : Y \rightarrow Y$ is called contraction mapping if there exists $\theta \in (0, 1)$ such that $\|Tx - Ty\| \leq \theta \|x - y\|$, for all $x, y \in Y$.

Example: $T : \mathbb{R}^n \rightarrow \mathbb{R}^n$ defined by $T(x) = \frac{1}{2}x$,here $\theta = \frac{1}{2}$

Definition1.17 **Nonexpansive mapping:** A mapping $T : Y \rightarrow Y$ is called nonexpansive mapping if $\|T x - T y\| \leq \|x - y\|$ for all $x, y \in Y$.

Example: $T : \mathbb{R}^n \rightarrow \mathbb{R}^n$ defined by $T(x) = x$,here $\theta = 1$

Definition1.18 **Quasi-nonexpansive mapping** : A mapping $T : Y \rightarrow Y$ is called quasi-nonexpansive mapping if for all $x \in Y$ and $p \in F(T)$, we have $\|T x - p\| \leq \|x - p\|$.

Example: $T : \mathbb{R}^n \rightarrow \mathbb{R}^n$ defined by $T(x) = x$,here $p \in \mathbb{R}^n$

Definition1.19 **Suzuki Condition (C) :** A mapping $T : Y \rightarrow Y$ is said to satisfy condition (C) if for all $x, y \in Y$, we have

$$\frac{1}{2}\|x - Tx\| \leq \|x - y\| \text{ implies } \|Tx - Ty\| \leq \|x - y\|$$

Example: $T : \mathbb{R}^n \rightarrow \mathbb{R}^n$ defined by $T(x) = \frac{1}{2}x$,here $\theta = \frac{1}{2}$

Definition1.110 Strong convergent : A sequence $\{x_n\}$ in a normed space X is said to be strong convergenc if there exist $x \in X$ such that

$$lim_{n\to\infty} ||x_n - x|| = 0$$

$$lim_{n\to\infty} x_n = x$$

Definition1.111 Weak Convergence : A sequence $\{x_n\}$ in a normed linear space X is said to be weak convergenc if there exist $x \in X$ such that for every $f \in X*$ (dual space)

$$lim_{n\to\infty} f(x_n) = f(x)$$

The element x is called weak limit of x_n & we say that x_n converges weakly to x.

Definition1.112 Convex set : A convex set defined as a set of point in which the line AB connecting any two points A,B in the set lies completely within that set.

Example 1: Empty sets, singleton set (x_0) .

Example 2: Euclidean ball $B(x_0, r) = \left\{x: \left||x - x_0|\right|_2 \le r\right\}$.

Definition1.113: Rate of Convergence: In the order of convergence and the rate of convergence of a convergent sequence are quantities that represent how quickly the sequence approaches its limit. A sequence (x_n) that converges to x* is said to have order of convergence $q \geq 1$ and rate of convergence μ if

$$lim_{n\to\infty} \frac{\|x_{n+1} - x^*\|}{\|x_n - x^*\|} q = \mu$$

The rate of convergence μ is also called the asymptotic error constant.

CHAPTER-2

Main Results

Some properties of non-expansive mapping that satisfies Suzuki condition(C)

Lemma1.1 Let $\{u_n\}_{n=0}^{\infty}$ and $\{v_n\}_{n=0}^{\infty}$ be two fixed point iteration procedure sequences that converge to the same fixed point p and $\|u_n - p\| \leq a_n$ and $\|v_n - p\| \leq b_n$ for all $n \geq 0$. If the sequences $\{a_n\}_{n=0}^{\infty}$ and $\{b_n\}_{n=0}^{\infty}$ converge to a and b, respectively, and $lim_{n\to\infty} \frac{\|a_n - a\|}{\|b_n - b\|} = 0$, then we say that $\{u_n\}_{n=0}^{\infty}$ converge faster than $\{v_n\}_{n=0}^{\infty}$ to p.

Lemma1.2 Let $\{t_n\}_{n=0}^{\infty}$ be an arbitrary sequence in Y. Then, an iteration procedure $x_{n+1} = f(T, x)$ converging to fixed point p, is said to be T-stable or stable with respect to T, if for $\varepsilon_n = \|t_{n+1} - f(T, t_n)\|$, $n = 0, 1, 2, 3\ldots\ldots$, we have $lim_{n\to\infty}\varepsilon_n = 0 \Longleftrightarrow lim_{n\to\infty} t_n = p$.

Lemma1.3 Let $T,\ T^* : X \to X$ be two operators. We say that $T^*$is an approximate operator for T if, for some $\varepsilon > 0$, we have

$$\|Tx - T^*x\| \leq \varepsilon, \qquad \text{for all } x \in X$$

Proposition 2.1. Let Y be a nonempty subset of a Banach space X and $T : Y \to Y$ be any mapping. Then

(i) If T is nonexpansive then T satisfies condition (C).

(ii) If T satisfies condition (C) and has a fixed point, then T is a quasi-nonexpansive mapping.

(iii) If T satisfies condition (C), then

$$\|x - Ty\| \leq 3\,\|Tx - x\| + \|x - y\| \text{ for all } x, y \in Y.$$

Lemma 2.2. Let T be a mapping on a subset Y of a Banach space X with the Opial property. Assume that T satisfies condition (C). If $\{x_n\}$ converges weakly to z and $lim_{n\to\infty}\|Tx_n - x_n\| = 0$, then $Tz = z$. That is, $I - T$ is demiclosed at zero.

Lemma 2.3. Let Y be a weakly compact convex subset of a uniformly convex Banach space X. Let T be a mapping on Y. Assume that T satisfies condition (C). Then T has a fixed point.

Lemma 2.4. Suppose that X is a uniformly convex Banach space and $\{t_n\}$ be any real sequence such that $0 < p \leq t_n \leq q < 1$ for all $n \geq 1$. Let $\{x_n\}$ and $\{y_n\}$ be any two senquences of X such that $limsup_{n\to\infty} \| x_n \| \leq r$, $limsup_{n\to\infty} \| y_n \| \leq r$ and $limsup_{n\to\infty} \| t_n x_n + (1-t_n) y_n = r$ hold for some $r \geq 0$. Then $lim_{n\to\infty} \| x_n - y_n \| = 0$ Let Y be a nonempty closed convex subset of a Banach space X, and let $\{x_n\}$ be a bounded sequence in X. For $x \in X$, we set $r(x, \{x_n\}) = limsup_{n\to\infty} \| x_n - x \|$.

Lemma 2.5. Let $\{\psi_n\}_{n=0}^{\infty}$ and $\{\phi_n\}_{n=0}^{\infty}$ be nonnegative real sequences satisfying the following inequality:
$\psi_{n+1} \leq (1 - \phi_n)\psi_n + \phi_n$, where $\phi_n \in (0,1)$, for all $n \in N$

$\sum_{n=0}^{\infty} \phi_n = \infty$ and $\frac{\psi_n}{\phi_n} \to 0$ as $n \to \infty$, then $lim_{n\to\infty}\psi_n = 0.$

Lemma 2.6. Let $\{\psi_n\}_{n=0}^{\infty}$ be nonnegative real sequences for which one assumes there exists $n_0 \in N$, such that for all $n \geq n_0$, the following inequality satisfies: $\psi_{n+1} \leq (1 - \phi_n)\psi_n + \psi_n \phi_n$, where $\phi_n \in (0, 1)$, for all $n \in N$, $\sum_{n=0}^{\infty} \phi_n = \infty$ and $\phi_n \geq 0$, for all $n \in N$, then
$0 \leq limsup_{n\to\infty} \psi_n \leq limsup_{n\to\infty} \phi_n$.

New k-iteration Process and its Convergence Analysis

- Through out this section we have $n \geq 0$ and $\{\alpha_n\}$ and $\{\beta_n\}$ are real sequences in $[0,1]$.

Gursoy and karakaya in introduced new iteration process called "**Picard-S iteration process",** as follow

$$\begin{aligned} u_0 &\in C \\ w_n &= (1 - \beta_n)u_n + \beta_n T u_n \\ v_n &= (1 - \alpha_n) T u_n + \alpha_n T w_n \\ u_{n+1} &= T v_n \qquad \textbf{(1*)} \end{aligned}$$

- They proved that the Picard-S iteration process can be used to approximate the fixed point of contraction mappings.

- Also, by providing an example, it is shown that the Picard-S iteration process converge faster than all Picard, Mann, Ishikawa, Noor, , Abbas, Normal-S and Two-step Mann iteration process.
- After this karakaya et. introduced a new two step iteration process, with the claim that it is even faster than Picard-S iteration process, as follow

$$\begin{aligned} u_0 &\in C \\ v_n &= T((1-\beta_n)u_n + \beta_n T u_n) \\ u_{n+1} &= T((1-\alpha_n)v_n + \alpha_n T\, v_n) \qquad \textbf{(2*)} \end{aligned}$$

Recently Thakur et. al. used the following new iteration process, we will call it ”Thakur New iteration process”,

$$\begin{aligned} u_0 &\in C \\ w_n &= (1-\beta_n)u_n + \beta_n T u_n \\ v_n &= T((1-\alpha_n)u_n + \alpha_n w_n) \\ u_{n+1} &= T v_n \qquad \textbf{(3*)} \end{aligned}$$

With the help of numerical example they proved that their new iteration process i.e.”Thakur New iteration process” is faster than Picard, Mann, Ishikawa, Agarwal, Noor and Abbas iteration process for some class of mappings

Problem 3.1. Is it possible to develop an iteration process whose rate of convergence is even faster than the iteration processes **(1*), (2*) and (3*)?**

: To answer this, we introduce the following new iteration process known as ”k Iteration Process”

$$\begin{aligned} x_0 &\in \mathrm{C} \\ z_n &= (1-\beta_n)\, x_n + \beta_n \mathrm{T} x_n \\ y_n &= \mathrm{T}((1-\alpha_n)\mathrm{T}x_n + \alpha_n \mathrm{T}\, z_n) \\ x_{n+1} &= \mathrm{T} y_n \qquad \textbf{(4*)} \end{aligned}$$

We will prove that our new iteration process **(4*)** is stable and have a good speed of convergence comparatively to other iteration processes. Also the data dependence result for fixed point of contraction mappings with the help of the new iteration process is proved.

Theorem 3.2. Let C be a nonempty closed convex subset of a Banach space X and T : C → C be a contraction mapping. Let$\{x_n\}_{n=0}^{\infty}$ be an iterative sequence generated by **(4*)** with real sequences $\{\alpha_n\}_{n=0}^{\infty}$and $\{\beta_n\}_{n=0}^{\infty}$ in [0, 1] satisfying $\sum_{n=0}^{\infty} \alpha_n\beta_n = \infty$. Then $\{x_n\}_{n=0}^{\infty}$ converge strongly to a unique fixed point of T.

Proof. The well-known Banach theorem guarantees the existence and uniqueness of fixed point p. We will show that $x_n \to$ p for $n \to \infty$. From **(4*)** we have

$$\begin{aligned}
\|z_n - p\| &= \|(1-\beta_n)\,x_n + \beta_n T x_n - (1-\beta_n+\beta_n)p\| \\
&\leq (1-\beta_n)\,\|x_n - p\| + \beta_n\,\|T\,x_n - Tp\| \\
&\leq (1-\beta_n)\,\|x_n - p\| + \beta_n\,\theta\,\|x_n - p\| \\
&= (1-\beta_n(1-\theta))\,\|x_n - p\|\,.
\end{aligned}$$

Similarly,

$$\begin{aligned}
\|y_n - p\| &= \|T((1-\alpha_n)T\,x_n + \alpha_n T\,z_n) - T\,p\| \\
&\leq \theta\,\|(1-\alpha_n)T\,x_n + \alpha_n T\,z_n - p\| \\
&\leq \theta[(1-\alpha_n)\,\|T\,x_n - p\| + \alpha_n\,\|T\,z_n - p\|] \\
&\leq \theta[(1-\alpha_n)\theta\,\|x_n - p\| + \alpha_n\theta\,\|z_n - p\|] \\
&\leq \theta^2[(1-\alpha_n)\,\|x_n - p\| + \alpha_n\|z_n - p\|] \\
&\leq \theta^2((1-\alpha_n)\,\|x_n - p\| + \alpha_n\,(1-\beta_n\,(1-\theta))\,\|x_n - p\|) \\
&\leq \theta^2(1-\alpha_n\beta_n\,(1-\theta))\,\|x_n - p\|\,. \qquad (6)
\end{aligned}$$

Hence

$$\begin{aligned}
\|x_{n-1} - p\| &= \|\mathrm{T}y_n - \mathrm{p}\| \\
&\leq \theta\,\|y_n - \mathrm{p}\| \\
&\leq \theta^3(1-\alpha_n\beta_n\,(1-\theta))\,\|x_n - p\|. \qquad (7)
\end{aligned}$$

Repetition of above processes gives the following inequalities

$$\begin{aligned}
\|x_{n+1} - p\| &\leq \theta^3(1-\alpha_n\beta_n\,(1-\theta))\,\|x_n - p\| \\
\|x_n - p\| &\leq \theta^3(1-\alpha_{n-1}\beta_{n-1}\,(1-\theta))\,\|x_{n-1} - p\| \\
\|x_{n-1} - p\| &\leq \theta^3\,(1-\alpha_{n-2}\beta_{n-2}\,(1-\theta))\,\|x_{n-2} - p\| \\
&\vdots
\end{aligned}$$

:

$$\|x_1 - p\| \leq \theta^3(1 - \alpha_0\beta_0 (1 - \theta)) \|x_0 - p\| \tag{8}$$

From (8) we can easily derive

$$\|x_{n+1} - p\| \leq \|x_0 - p\| \theta^{3(n+1)} \prod_{k=0}^{n}(1 - \alpha_k\beta_k(1 - \theta)), \tag{9}$$

where $1 - \alpha_k\beta_k(1 - \theta) < 1$, because $\theta \in (0, 1)$ and α_n, $\beta_n \in [0, 1]$, for all $n \in N$. Since we know that $1 - x \leq e^{-x}$ for all $x \in [0, 1]$, so from (9) we get

$$\|x_{n+1} - p\| \leq \|x_0 - p\| \theta^{3(n+1)} e^{-(1-\theta)\sum_{k=0}^{n}\alpha_k\beta_k}. \tag{10}$$

Taking the limit of both sides of (10), we get $\lim_{n\to\infty}\|x_n - p\| = 0$, i.e. $x_n \to p$ for $n \to \infty$, as required.

Theorem 3.3. Let C be a nonempty closed convex subset of a Banach space X and $T : C \to C$ be a contraction mapping. Let $\{x_n\}_{n=0}^{\infty}$ be an iterative sequence generated by **(4*)** with real sequences $\{\alpha_n\}_{n=0}^{\infty}$ and $\{\beta_n\}_{n=0}^{\infty}$ in [0, 1] satisfying $\sum_{n=0}^{\infty}\alpha_n\beta_n = \infty$. Then the iterative process **(4*)** is **T**-stable.

Proof. Let $\{t_n\}_{n=0}^{\infty} \subset X$ be any arbitrary sequence in C. Let the sequence generated by **(4*)** is $x_{n+1}= f(T, x_n)$ converging to unique fixed point p **(by Theorem 3.2)** and $\varepsilon_n= \|t_{n+1} - f(T, t_n)\|$.
We will prove that $lim_{n\to\infty}\, \varepsilon_n= 0 \Longleftrightarrow lim_{n\to\infty}t_n= p.$

Let $lim_{n\to\infty}\varepsilon_n= 0$, we have

$$\begin{aligned}\|t_{n+1} - p\| &\leq \|t_{n+1} - f(T, t_n)\| + \|f(T, t_n) - p\| \\ &= \varepsilon_n + \|T(T((1 - \beta_n)Tt_n + \beta_n T((1 - \alpha_n)\, t_n + \alpha_n Tt_n))) - p\| \\ &\leq \theta^3(\,(1 - \alpha_n\beta_n\,(1 - \theta))\, \|t_n - p\| + \varepsilon_n.\end{aligned}$$

Since $\theta \in (0, 1)$, α_n, $\beta_n \in [0, 1]$, for all $n \in N$ and $lim_{n\to\infty}\varepsilon_n= 0$, so the above inequality together with **Lemma 2.8** leads to $lim_{n\to\infty}\|t_n - p\| = 0$. Hence $lim_{n\to\infty}t_n= p$. Conversely let $lim_{n\to\infty}t_n= p$, we have

$$\begin{aligned}\varepsilon_n &= \|t_{n+1} - f(T, t_n)\| \\ &\leq \|t_{n+1} - p\| + \|f(T, t_n) - p\| \\ &\leq \|t_{n+1} - p\| + \theta^3(\,(1 - \alpha_n\beta_n\,(1 - \theta))\, \|t_n - p\| .\end{aligned}$$

This implies that $lim_{n\to\infty}\varepsilon_n = 0$. Hence **(4*)** is stable with respect to T.

Theorem 3.4. Let C be a nonempty closed convex subset of a Banach space X and T : C → C a contraction mapping with fixed point p.
For given $u_0 = x_0 \in C$, let $\{u_n\}_{n=0}^{\infty}$ and $\{x_n\}_{n=0}^{\infty}$ be an iterative sequences generated by **(1*)** and **(4*)** respectively, with real sequences $\{\alpha_n\}_{n=0}^{\infty}$ and $\{\beta_n\}_{n=0}^{\infty}$ in [0, 1] satisfying (i). $\alpha \leq \alpha_n < 1$ and $\beta \leq \beta_n < 1$, for some $\alpha, \beta > 0$ and for all $n \in N$. Then $\{x_n\}_{n=0}^{\infty}$ converge to p faster than $\{u_n\}_{n=0}^{\infty}$ does.

Proof. From (9) of Theorem 3.2, we have

$$\|x_{n+1} - p\| \leq \|x_0 - p\| \, \theta^{3(n+1)} \prod_{k=0}^{n}(1 - \alpha_k \beta_k (1 - \theta)), \tag{11}$$

The following inequality is due to [(7),(2.5)] which is obtained from (1), also converging to unique fixed point p

$$\|u_{n+1} - p\| \leq \|u_0 - p\| \theta^{2(n+1)}) \prod_{k=0}^{n}(1 - \alpha_k \beta_k (1 - \theta)), \tag{12}$$

Together with assumption (i), (11) implies that,

$$\begin{aligned} \|x_{n+1} - p\| &\leq \|x_0 - p\| \, \theta^{3(n+1)} \prod_{k=0}^{n}(1 - \alpha\beta(1 - \theta)), \\ &\leq \|x_0 - p\| \, \theta^{3(n+1)} (1 - \alpha\beta(1 - \theta))^{n+1} . \end{aligned} \tag{13}$$

Similarly (12) together with assumption (i) leads to,

$$\begin{aligned} \|u_{n+1} - p\| &\leq \|u_0 - p\| \theta^{2(n+1)} \prod_{k=0}^{n}(1 - \alpha\beta(1 - \theta)), \\ &\leq \|u_0 - p\| \, \theta^{2(n+1)} (1 - \alpha\beta(1 - \theta))^{n+1} . \end{aligned} \tag{14}$$

Define

$a_n = \|x_0 - p\| \, \theta^{3(n+1)} (1 - \alpha\beta(1 - \theta))^{n+1}$, and

$b_n = \|u_0 - p\| \, \theta^{2(n+1)} (1 - \alpha\beta(1 - \theta))^{n+1}$, then

$$\Psi n = \frac{a_n}{b_n}$$

$$= \frac{\|x_0 - p\| \, \theta^{3(n+1)} (1 - \alpha\beta(1 - \theta))^{n+1}}{\|u_0 - p\| \, \theta^{2(n+1)} (1 - \alpha\beta(1 - \theta))^{n+1}} = \theta^{n+1} . \tag{15}$$

Since $lim_{n\to\infty} \frac{\Psi_{n+1}}{\Psi_n} = lim_{n\to\infty} \frac{\theta^{n+2}}{\theta^{n+1}} = \theta < 1$, so by ratio test $\sum_{n=0}^{\infty} \Psi_n < \infty$. Hence from (15) we have,

$lim_{n\to\infty} \frac{a_n}{b_n} = lim_{n\to\infty} \Psi_n = 0$, which implies that $\{x_n\}_{n=0}^{\infty}$ is faster than $\{u_n\}_{n=0}^{\infty}$.

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C operators are the symbols that are used in C programs to perform mathematical and logical operations. C operators combine variables and constants to create expressions. To form expressions, operators, functions, constants, variables and operators are combined.

In the expression X +Y *20. **"+"," *"** and operators **X, Y are variables, 20 is constant, and X +Y *20 is an expression.**

In this post we will look into special operators in C. But let's first see what are the other types of operators does C provide.

Types of Operators in C

C provides 6 types of built-in operators:

1. **Arithmetic Operators** : This includes +, -, *, /, %, *post-increment, pre-increment, post-decrement, pre-decrement*
2. **Relational Operators** : This includes ==, !=, >, <, >= and <=
3. **Logical Operators** : This includes &&, || and !
4. **Bitwise Operators** : This includes &, |, ^, ~, >> and <<
5. **Assignment Operators** : This includes =, +=, -=, *=, etc.
6. **Special Operators** : This includes cast operator, comma, sizeof, reference, dereference, double pointer

Arithmetic Operator In C

Arithmetic operator in C can be divided into two types:

1. **Unary Operator:** This kind of operators needs only one operand like ++ and —
2. **Binary Operator:** This kind of operators requires at-least two operand like +,* etc.

The Arithmetic Operators are described below:

Operator	Description	Example
Addition	The '+' operator is used to perform addition of two operands	x+y

Subtraction	The '-' operator is used to perform subtraction of two operands	x-y
Multiplication	The '*' operator is used to perform multiplication of two operands	x*y
Division	The '/' operator is used to divide the first operand by the second	x/y
Modulus	The '%' operator returns the remainder when first operand is divided by the second	x%y
Increment	The '++' operator is used to increment number by one. It can be post or pre increment	++x, x++
Decrement	The '–'operator is used to decrement number by one. It can be post or pre decrement	–x, x–

```
// Arithmetic Operator In C
#include <stdio.h>
int main()
{
int a = 10,b = 12, c;
c = a+b;
printf("Addition of a and b = %d \n",c);
c = a-b;
printf("Subtraction of a and b = %d \n",c);
c = a*b;
printf("Multiplication of a and b = %d \n",c);
c = a/b;
printf("Division of a and b = %d \n",c);
```

```
c = a%b;
printf("Remainder when a divided by b = %d \n",c);
printf("Value of a after increment = %d \n", ++a);
printf("Value of b after decrement = %d \n", --b);
return 0;
}
```

Output

```
Addition of a and b = 22

Subtraction of a and b = -2

Multiplication of a and b = 120

Division of a and b = 0

Remainder when a divided by b = 10

Value of a after increment = 11

Value of b after decrement = 11
```

Relational Operators in C

Operator	Description	Example
Equal To ==	Checks whether the two given operands are equal or not. If yes, it returns true else false	x==y
Not Equal To !=	Checks whether the two given operands are equal or not. If not, it returns true else false.	x!=y

Greater Than >	Checks whether the first operand is greater than the second operand or not.	x>y
Less Than <	Checks whether the first operand is lesser than the second operand.	x<y
Greater than or equal to >=	Checks whether the first operand is greater than or equal to the second operand.	x>=y
Less than or equal to <=	Checks whether the first operand is less than or equal to the second operand.	x<=y

```
//Relational Operators in C

#include<stdio.h>

int main()
{
    int x = 20, y = 30;

    printf("x = %d\n", x);
    printf("y = %d\n", y);

    // Check if x is greater than y
    printf("Is x > y : %d\n", x > y);

    // Check if x is greater than or equal to y?
    printf("Is x >= y : %d\n", x >= y);

    // Check if x is smaller than y?
    printf(" Is x < y : %d\n", x < y);

    // Check if x is smaller than or equal to y?
    printf("Is x <= y : %d\n", x <= y);
```

```
    // Check if x is equal to y?
    printf("Is x == y : %d\n", x == y);

    // Check if x is not equal to y?
    printf("Is x != y : %d\n", x != y);

    return 0;
}
```

Output

```
x = 20

y = 30

Is x > y : 0

Is x >= y : 0

Is x < y : 1

Is x <= y : 1

Is x == y : 0

Is x != y : 1
```

Logical Operators in C

Operator	Description	Example
Logical AND &&	This operator returns true when both the conditions which are compared are true.	a && b

Logical OR ||	This operator returns true when any one of the conditions which are compared are true.	x-y
Logical NOT !	The '*' operator multiplies two operands	X*y

```
#include <stdio.h>
int main()
{
    int a = 5, b = 5, c = 10, result;

   //This will be true when both conditions are true
    result = (a == b) && (c > b);
    printf("(a == b) && (c > b) is %d \n", result);
    result = (a == b) && (c < b);
    printf("(a == b) && (c < b) is %d \n", result);

    //This will be true when either one of the condition are true
    result = (a == b) || (c < b);
    printf("(a == b) || (c < b) is %d \n", result);
    result = (a != b) || (c < b);
    printf("(a != b) || (c < b) is %d \n", result);

   // Negates the output
    result = !(a == b);
    printf("!(a == b) is %d \n", result);

    return 0;
}
```

Output

```
(a == b) && (c > b) is 1
(a == b) && (c < b) is 0
(a == b) || (c < b) is 1
(a!= b) || (c < b) is 0
!(a == b) is 0
```

Bitwise Operators in C

Operator	**Description**	**Example**
bitwise AND &	This operator takes two numbers as operands and does AND on every bit of two numbers. The result of AND is 1 only if both bits are 1	x & y
bitwise OR |	This operator takes two numbers as operands and does OR on every bit of two numbers. The result of OR is 1 only if any of the bit is 1	x | y
bitwise XOR ^	This operator takes two numbers as operands and does XOR on every bit of two numbers. The result of XOR is 1 only if two bits are different	x ^ y
Left Shift <<	This operator takes two numbers and does left shift of the bits of the first operand where the second operand decides the number of places to be shifted	x<<4
Right Shift >>	This operator takes two numbers and does right shift of the bits of the first operand where the second operand decides the number of places to be shifted	x>>4
bitwise NOT ~	This operator takes one number and inverts all bits of it	!x

Assignment Operators in C

Operator	**Description**	**Example**

=	This operator is used to assign the value on the right to the variable on the left	X=5
+=	This operator first adds the current value of the variable on left to the value on the right and then assigns the result to the variable on the left.	x+=7
-=	This operator first subtracts the current value of the variable on left from the value on the right and then assigns the result to the variable on the left.	x-=7
*=	This operator first multiplies the current value of the variable on left from the value on the right and then assigns the result to the variable on the left	x*=7
/=	This operator first divides the current value of the variable on left from the value on the right and then assigns the result to the variable on the left	x/=7

Math Functions

There is also a list of math functions available, that allows you to perform mathematical tasks on numbers. To use them, you must include the math.h **header file** in your program:

```
#include <math.h>
```

Square Root

To find the square root of a number, use the sqrt() function:

Example

```
printf("%f", sqrt(16));
```

Round a Number

The ceil() function rounds a number upwards to its nearest integer, and the floor() method rounds a number downwards to its nearest integer, and returns the result:

Example

```
printf("%f", ceil(1.4));
printf("%f", floor(1.4));
```

Power

The pow() function returns the value of x to the power of y (x^y):

Example

```
printf("%f", pow(4, 3));
```

Other Math Functions

A list of other popular math functions (from the <math.h> library) can be found in the table below:

Function	**Description**
abs(x)	Returns the absolute value of x
cos(x)	Returns the cosine of x
exp(x)	Returns the value of E^x
sin(x)	Returns the sine of x (x is in radians)
tan(x)	Returns the tangent of an angle

- **int sin(int)** : This function takes angle (in radian) as an argument and return its sine value that could be verified using sine curve.
- **int cos(int)** : This function takes angle (in radian) as an argument and return its cosine value that could be verified using cosine curve.
- **int tan(int)** : This function takes angle (in radian) as an argument and return its tangent value. This could also be verified using Trigonometry as Tan(x) = Sin(x)/Cos(x).

- **int sqrt(int)** : This function takes number as an argument and return its square root value. Number cannot be negative value.
- **int abs(int)** : This function takes integer number as an argument and return its absolute value. It means, the output will always be positive regardless of sign of input.
- **int pow(int, int)** : This function takes one argument as base and other as exponent.
- **int floor(int)** : This functions returns the integer value lesser or equal to argument passed in the function.
- **int fabs(int)** : This function returns the absolute value of any number.
- **int log(int)** : This function takes a number and returns the natural log of that number.

Control Structures

if else Statement

The if-else statement in C is used to perform the operations based on some specific condition. The operations specified in if block are executed if and only if the given condition is true.
There are the following variants of if statement in C language.

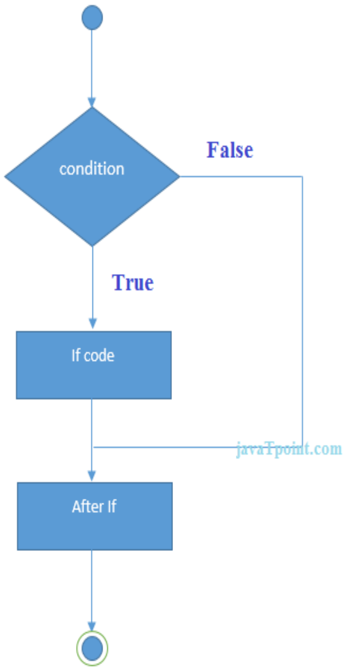
- If statement
- If-else statement
- If else-if ladder
- Nested if

If Statement

The if statement is used to check some given condition and perform some operations depending upon the correctness of that condition. It is mostly used in the scenario where we need to perform the different operations for the different conditions. The syntax of “if statement is given below”.

```
if(expression)

{

    //code to be executed

}
```

Flowchart of if statement in C



```
#include<stdio.h>
int main()
{
int number=0;
printf("Enter a number:");
scanf("%d",&number);
if(number%2==0){
printf("%d is even number",number);
}
return 0;
}
```

Output

```
Enter a number:4

4 is even number

Enter a number:5
```

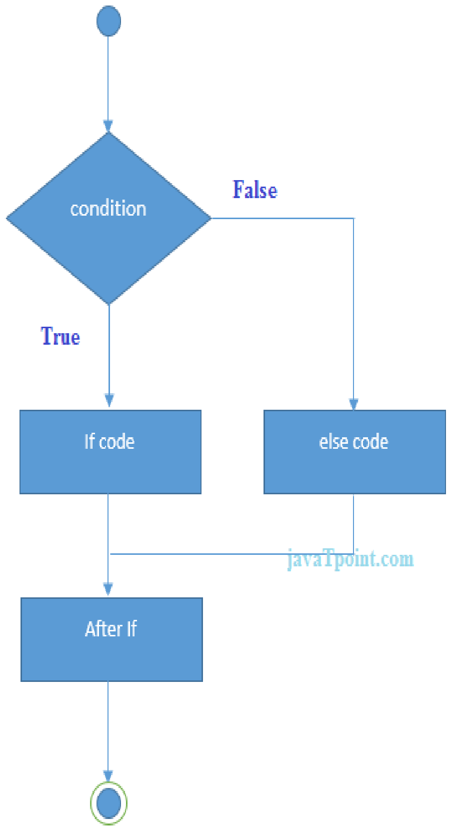
If-else Statement

The if-else statement is used to perform two operations for a single condition. The if-else statement is an extension to the if statement using which, we can perform two different operations, i.e., one is for the correctness of that condition, and the other is for the incorrectness of the condition. Here, we must notice that if and else block cannot be executed simultaneously. Using if-else statement is always preferable since it always invokes an otherwise case with every if condition.

The syntax of the if-else statement is given below.

```
if(expression)

{

//code to be executed if condition is true

}else{

//code to be executed if condition is false

}
```

Flowchart of the if-else statement in C



```
#include<stdio.h>
int main()
{
int number=0;
printf("enter a number:");
scanf("%d",&number);
if(number%2==0)
{
printf("%d is even number",number);
}
else
{
printf("%d is odd number",number);
}
return 0;
}
```

Output

```
enter a number:4

4 is even number

enter a number:5

5 is odd number
```

else-if ladder Statement

The if-else-if ladder statement is an extension to the if-else statement. It is used in the scenario where there are multiple cases to be performed for different conditions. In if-else-if ladder statement, if a condition is true then the statements defined in the if block will be executed, otherwise if some other condition is true then the statements defined in the else-if block will be executed, at the last if none of the condition is true then the statements defined in the else block will be executed. There are multiple else-if blocks possible. It is similar to the switch case statement where the default is executed instead of else block if none of the cases is matched.

```
if(condition1)
{
//code to be executed if condition1 is true
}else if(condition2){
//code to be executed if condition2 is true
}
else if(condition3){
//code to be executed if condition3 is true
}
...
else{
//code to be executed if all the conditions are false
}
```

Flowchart of else-if ladder statement in C

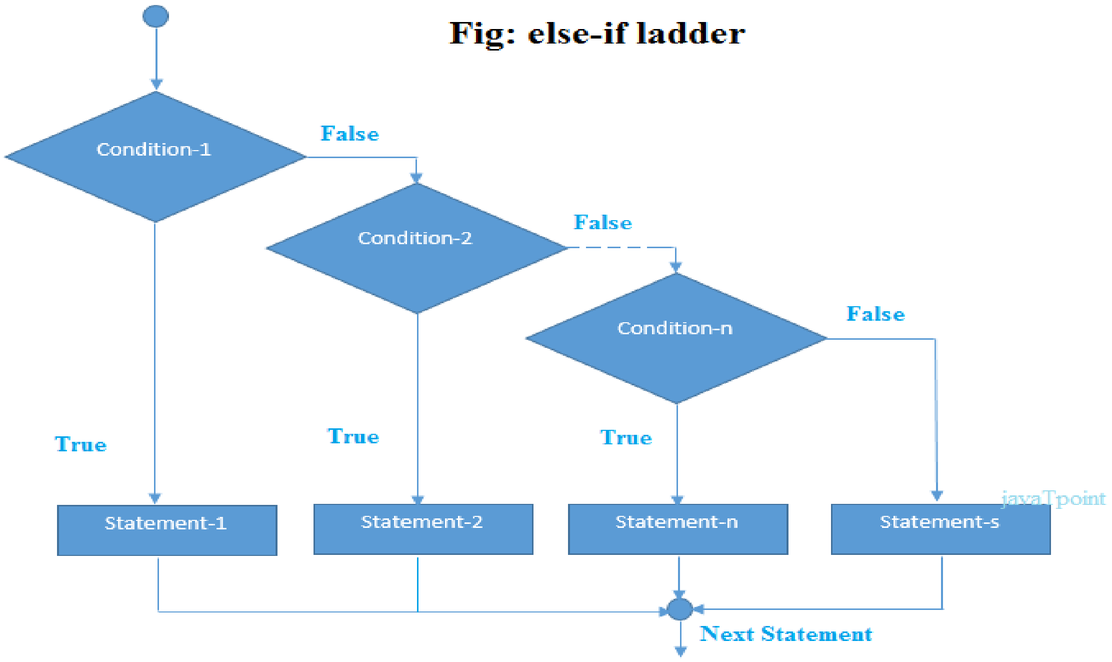


Fig: else-if ladder

Example

```
#include<stdio.h>
int main()
{
int number=0;
printf("enter a number:");
scanf("%d",&number);
if(number==10)
{
printf("number is equals to 10");
}
else if(number==50){
printf("number is equal to 50");
}
else if(number==100)
{
printf("number is equal to 100");
}
```

```
else
{
printf("number is not equal to 10, 50 or 100");
}
return 0;
}
```

Output

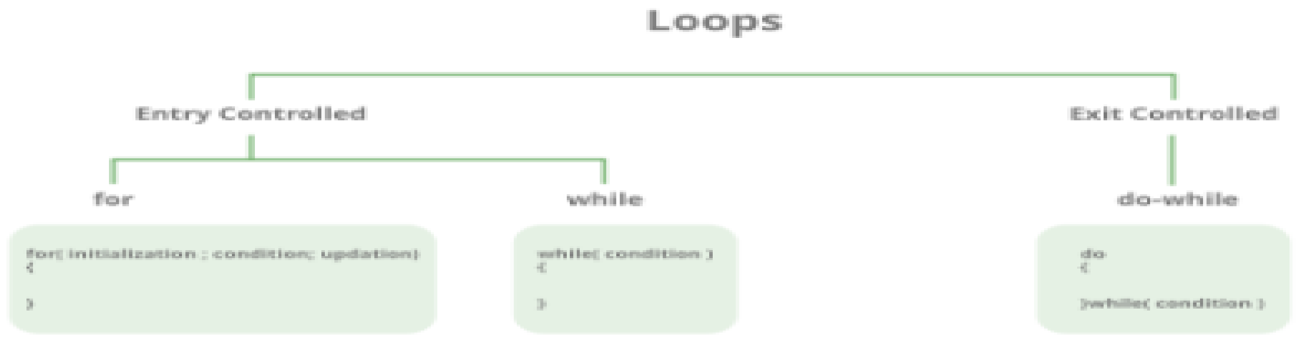
```
enter a number:4
number is not equal to 10, 50 or 100
enter a number:50
number is equal to 50
```

Loops

Loops in programming are used to repeat a block of code until the specified condition is met. A loop statement allows programmers to execute a statement or group of statements multiple times without repetition of code.

There are mainly two types of loops in C Programming:

1. **Entry Controlled loops:** In Entry controlled loops the test condition is checked before entering the main body of the loop. **For Loop and While Loop** is Entry-controlled loops.
2. **Exit Controlled loops:** In Exit controlled loops the test condition is evaluated at the end of the loop body. The loop body will execute at least once, irrespective of whether the condition is true or false. **do-while Loop** is Exit Controlled loop.



```
for( initialization ; condition; updation)
{

}
```

```
while( condition )
{

}
```

```
do
{

}while( condition )
```

Loop Type	Description
for loop	first Initializes, then condition check, then executes the body and at last, the update is done.

Loop Type	Description
while loop	first Initializes, then condition checks, and then executes the body, and updating can be inside the body.
do-while loop	do-while first executes the body and then the condition check is done.

for Loop

for loop in C programming is a repetition control structure that allows programmers to write a loop that will be executed a specific number of times. for loop enables programmers to perform n number of steps together in a single line.

Syntax:

```
for (initialize expression; test expression; update expression)

{

    //

    // body of for loop

    //

}
```

Example:

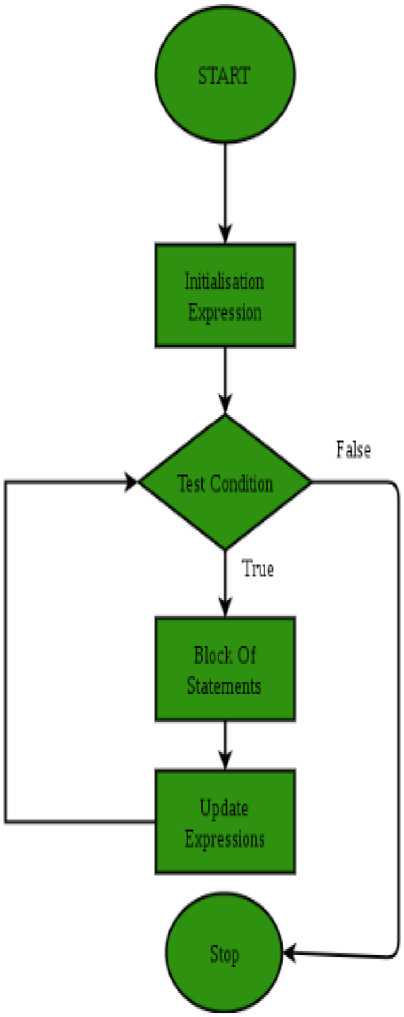
```
for(i=0;i<n;++i)

{

    printf("Body of for loop which will execute till n");

}
```

In for loop, a loop variable is used to control the loop. Firstly we initialize the loop variable with some value, then check its test condition. If the statement is true then control will move to the body and the body of for loop will be executed. Steps will be repeated till the exit condition becomes true. If the test condition will be false then it will stop.

- **Initialization Expression:** In this expression, we assign a loop variable or loop counter to some value. for example: int i=1;
- **Test Expression:** In this expression, test conditions are performed. If the condition evaluates to true then the loop body will be executed and then an update of the loop variable is done. If the test expression becomes false then the control will exit from the loop. for example, i<=9;

- **Update Expression:** After execution of the loop body loop variable is updated by some value it could be incremented, decremented, multiplied, or divided by any value.

for loop Equivalent Flow Diagram: example output



```
// C program to illustrate for loop
#include <stdio.h>

// Driver code

int main()

{

int i = 0;

for (i = 1; i <= 10; i++)

{

        printf( "Hello World\n");

}

return 0;

}
```

Output

```
Hello World

Hello World

Hello World

Hello World

Hello World

Hello World

Hello World

Hello World

Hello World

Hello World
```

While Loop

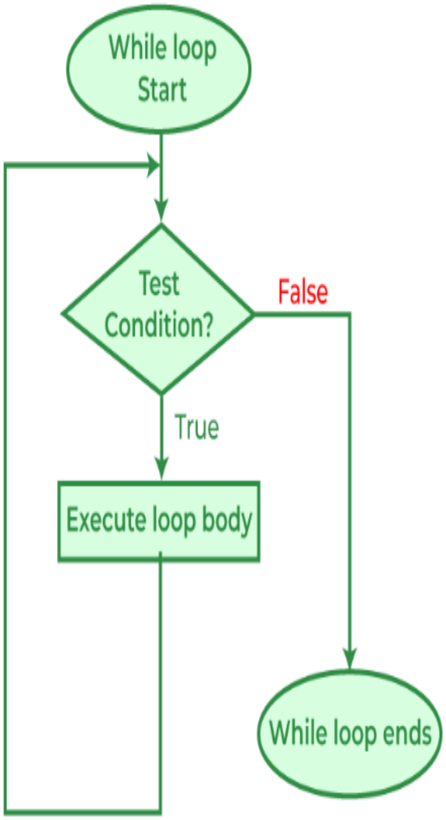
While loop does not depend upon the number of iterations. In for loop the number of iterations was previously known to us but in the While loop, the execution is terminated on the basis of the test condition. If the test condition will become false then it will break from the while loop else body will be executed.

Syntax:

```
initialization_expression;

while (test_expression)

{

    // body of the while loop

    update_expression;
```

}

Flow Diagram for while loop:



```
// C program to illustrate
// while loop
#include <stdio.h>
// Driver code
int main()
{
// Initialization expression
int i = 2;

// Test expression
while(i < 10)
{
// loop body
printf( "Hello World\n");
// update expression

        i++;
}
return 0;
}
```

```
Output
Hello World
Hello World
Hello World
Hello World
Hello World
Hello World
Hello World
Hello World
```

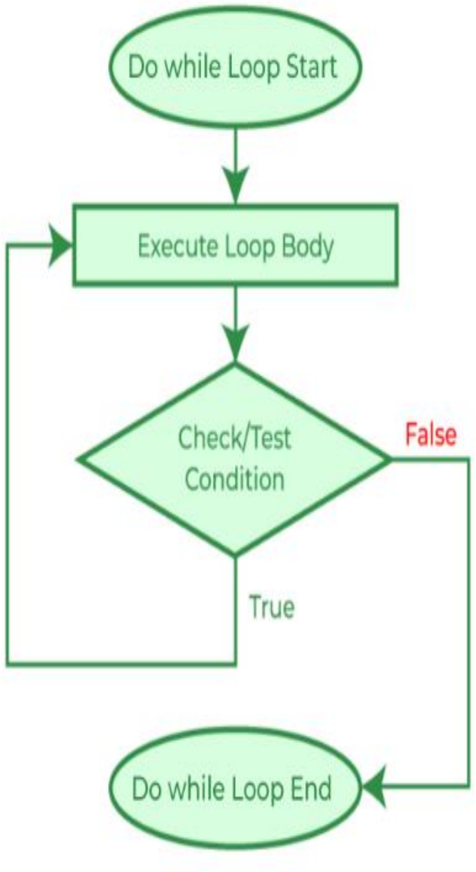
do-while Loop

The do-while loop is similar to a while loop but the only difference lies in the do-while loop test condition which is tested at the end of the body. In the do-while loop, the loop body will **execute at least once** irrespective of the test condition.

Syntax:

```
initialization_expression;

do
{
   // body of do-while loop
   update_expression;

} while (test_expression);
```

Flow diagram example and output



```
// C program to illustrate
// do-while loop
#include <stdio.h>

// Driver code
int main()
{
// Initialization expression
int i = 2;

do
{
		// loop body
		printf( "Hello World\n");

		// Update expression
		i++;

		// Test expression
} while (i < 1);

return 0;
}
```

OUTPUT

```
Hello World
```

Nested for Loop

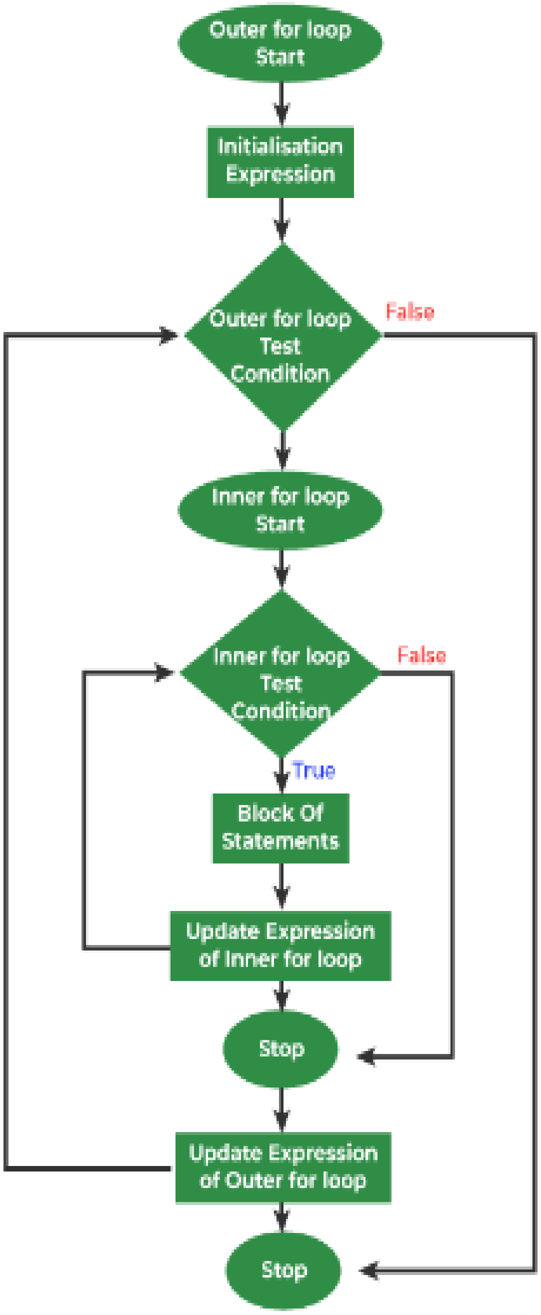
Nested for loop refers to any type of loop that is defined inside a ‘for’ loop. Below is the equivalent flow diagram for nested ‘for’ loops.

Syntax:

```
for ( initialization; condition; increment )
 {

   for ( initialization; condition; increment )
{
```

```
      // statement of inside loop
 }

   // statement of outer loop
}
```

FLOW DIAGRAM EXAMPLE AND OUTPUT



```
// C program to print elements of Three-Dimensional Array
// with the help of nested for loop
#include <stdio.h>
int main()
{
// initializing the 3-D array
int arr[2][3][2]= { { { 0, 6 }, { 1, 7 }, { 2, 8 } },{ { 3, 9 }, { 4, 10 }, { 5, 11 } }};
// Printing values of 3-D array
for (int i = 0; i < 2; ++i) {
for (int j = 0; j < 3; ++j) {
for (int k = 0; k < 2; ++k) {
printf("Element at arr[%i][%i][%i] = %d\n",i, j, k, arr[i][j][k]);
}
}
}
return 0;
}
```

OUTPUT

```
Element at arr[0][0][0] = 0

Element at arr[0][0][1] = 6

Element at arr[0][1][0] = 1

Element at arr[0][1][1] = 7

Element at arr[0][2][0] = 2

Element at arr[0][2][1] = 8

Element at arr[1][0][0] = 3

Element at arr[1][0][1] = 9

Element at arr[1][1][0] = 4

Element at arr[1][1][1] = 10

Element at arr[1][2][0] = 5

Element at arr[1][2][1] = 11
```

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Topic

Organometallic compounds

By

Miss. S.G. Vader

Introduction:

- Organometallic compounds are chemical compounds that contain a bond between a carbon atom and a metal.
- They are a cross between organic and inorganic chemistry and have many applications in industrial processes and clinical settings.
- Examples of organometallic compounds:
- Organomagnesium compounds, such as MeMgI iodomethylmagnesium and (diethylmagnesium)
- Organolithium compounds, such as BuLi (butyllithium)
- Organozinc compounds, such as ClZnCHC(= O)O Et) chloro(ethoxycarbonylmethyl)zinc
- Lithium dimethylcuprate, Li(CuMe)
- Triethylborane, EtB

Importantance of organometallic compounds:

- Catalysis
- They are used as catalysts in many reactions, increasing the rate of reactions and leading to more efficient use of reagents and energy. For example, rhodium complexes are used in the manufacture of medications like levodopa, which is used to treat Parkinson's disease.

- Medicine
- Organometallic compounds have unique properties that make them useful in medicinal chemistry. Some organometallic compounds have already entered clinical trials.

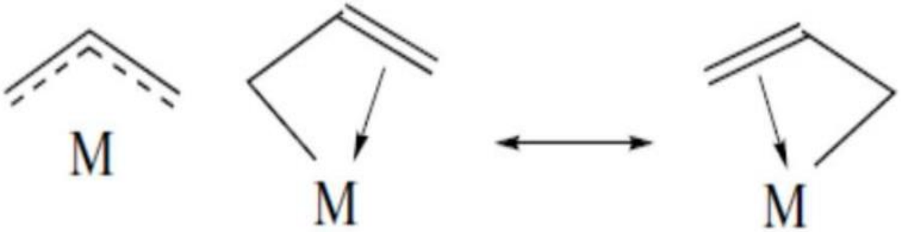
- Materials
- Organometallic compounds are used in the preparation of nanomaterials and microelectronic materials, such as thin films in integrated circuits. Silicon-based organometallic compounds are water repellent, heat stable, and resistant to chemical attack.

- **Chemical bonding:**
- Organometallic compounds have unique bonds and structures that have helped advance the understanding of chemical bonding.
- **Scientific inquiry:**
- Organometallic chemistry is full of intriguing stories of scientific discovery. Exploring how researchers take a new organometallic reaction from “ooh pretty” to strong predictive power is instructive for anyone interested in “how science works”.

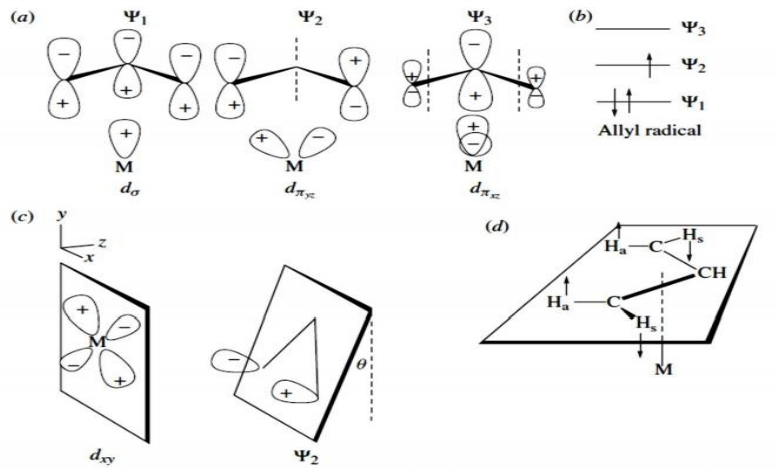
Structure and bonding in metal allyl complexes:

- Bonding and Electronic Features
- The allyl group commonly behaves as an actor ligand,coordinate with metals in one of two ways.
- In the monohapto form it is a simple 1e X-type ligand like Me.
- In the trihapto form, it acts as a 3e LX enyl ligand.
- This bonding mode can exist in two canonical forms.
- Intermediate cases between monohapto and trihapto forms ($\eta2$-allyls) are also known

Canonical forms:



Pictorial representation of bonding:



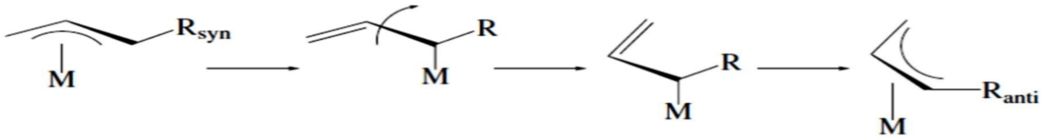
The electronic structure of the allyl ligand and some features of metal-allyl bonding. Nodes are shown as dotted lines in (a)

Bonding:

- Figure (a) in the previous slide display that of the three molecular orbitals of the allyl fragment.
- ψ1can interact with a suitable metal dσ orbital
- ψ2 with an M(dπ) orbital on the metal;
- • Ψ3 is not a frontier orbital and so probably of lesser importance.
- As the number of nodes increases, the MOs of the free ligand become less stable(b).
- Two peculiarities of the structures of η3
- -allyl complexes can be understood on this picture.

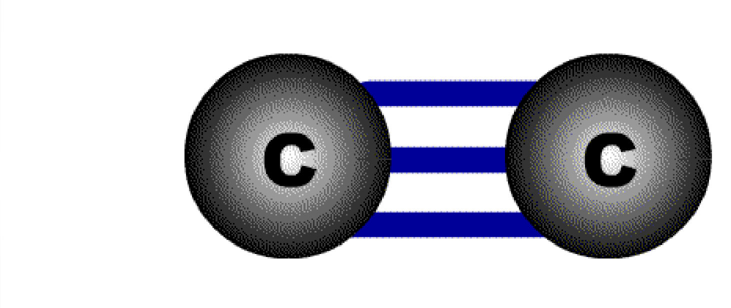
- First, the plane of the allyl is canted at an angle θ with respect to the
- coordination polyhedron around the metal, as shown in Fig. c; θ is usually 5◦–10◦
- • The reason is that the interaction between ψ2 and the dxy orbital on the metal is lmproved if the allyl group moves in this way, as can be seen in Fig. c.
- The structures also show that the terminal CH2 groups of the allyl are twisted about the C−C vector so as to rotate the anti hydrogens, Ha away from the metal, and the syn hydrogens, Hs, toward the metal as shown by the arrows in Fig. d.
- • This allows the p orbital on these carbons to point more directly toward the
- metal, thus further improving the overlap. Note the nomenclature of the allyl
- substituents, which are syn or anti with respect to the central CH

- The η3 allyl group often shows exchange of the syn and anti
- substituents. One mechanism goes through an η1-allylintermediate. This kind of exchange can affect the appearanceof the 1H NMR spectrum and also means that an allyl complexof a given stereochemistry may rearrange with time.



References:

- Basic Organometallic Chemistry: Concepts,Syntheses and Applications by B. D. Gupta andAnil J. Elias
- The Organometallic Chemistry of the Transition Metals by R. H. Crabtree



Infrared Spectroscopy

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IR Spectroscopy

I. Introduction

A. **Spectroscopy** is the study of the interaction of matter with the electromagnetic spectrum

1. Electromagnetic radiation displays the properties of both particles and waves

2. The particle component is called a ***photon***

3. The energy (**E**) component of a photon is proportional to the frequency. Where **h** is Planck's constant and ν is the frequency in Hertz (cycles per second)

$$\mathbf{E = h\nu}$$

4. The term "photon" is implied to mean a small, massless particle that contains a small wave-packet of EM radiation/light – we will use this terminology in the course

IR Spectroscopy

I. Introduction

5. Because the speed of light, ***c***, is constant, the ***frequency, ν***, (number of cycles of the wave per second) can complete in the same time, must be inversely proportional to how long the oscillation is, or ***wavelength***:

$$\nu = \frac{c}{\lambda} \qquad\qquad ⍰\; E = h\nu = \frac{hc}{\lambda}$$

$$c = 3 \times 10^{10} \text{ cm/s}$$

6. Amplitude, ***A***, describes the wave height, or strength of the oscillation

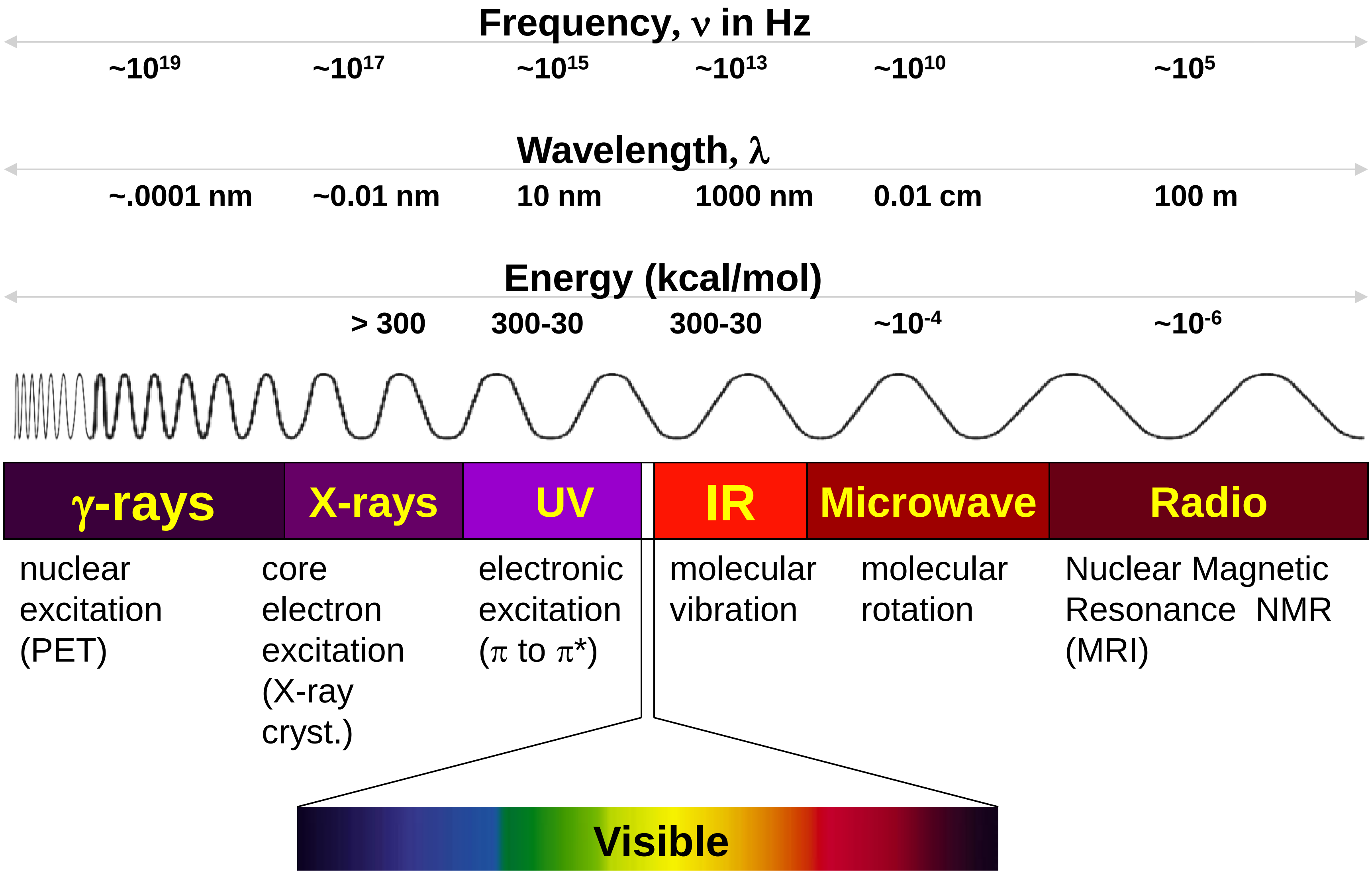
7. Because the atomic particles in matter also exhibit wave and particle properties (though opposite in how much) EM radiation can interact with matter in two ways:
   - Collision – particle-to-particle – energy is lost as heat and movement

   - Coupling – the wave property of the radiation matches the wave property of the particle and "couple" to the next higher quantum mechanical energy level

IR Spectroscopy

I. Introduction

8. The entire electromagnetic spectrum is used by chemists:



	γ-rays	**X-rays**	**UV**	**IR**	**Microwave**	**Radio**
Frequency, ν in Hz	**~10^{19}**	**~10^{17}**	**~10^{15}**	**~10^{13}**	**~10^{10}**	**~10^{5}**
Wavelength, λ	**~.0001 nm**	**~0.01 nm**	**10 nm**	**1000 nm**	**0.01 cm**	**100 m**
Energy (kcal/mol)		**> 300**	**300-30**	**300-30**	**~10^{-4}**	**~10^{-6}**
	nuclear excitation (PET)	core electron excitation (X-ray cryst.)	electronic excitation (π to π*)	molecular vibration	molecular rotation	Nuclear Magnetic Resonance NMR (MRI)

Visible

IR Spectroscopy

I. Introduction

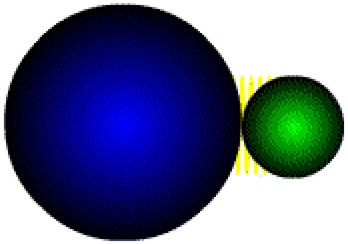
C. The IR Spectroscopic Process

1. The quantum mechanical energy levels observed in IR spectroscopy are those of ***molecular vibration***

2. We perceive this vibration as heat

3. When we say a ***covalent bond*** between two atoms is of a certain length, we are citing an average because the bond behaves as if it were a vibrating spring connecting the two atoms

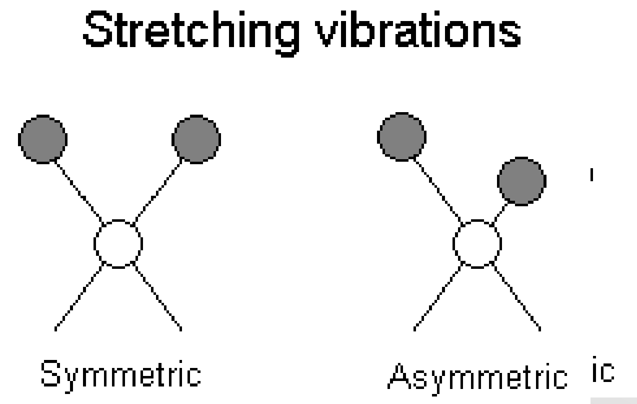
4. For a simple diatomic molecule, this model is easy to visualize:

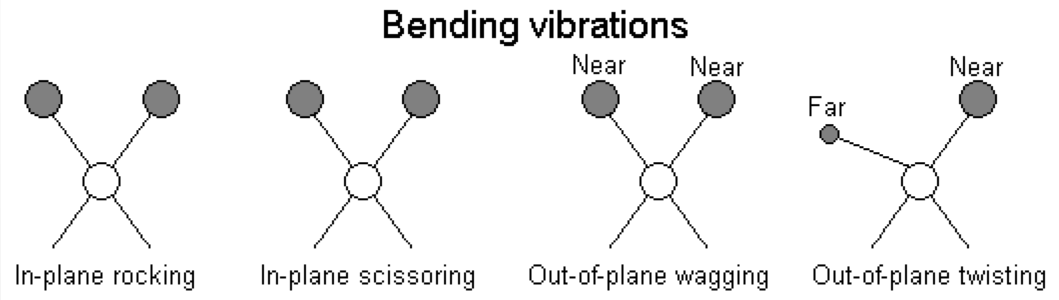


Vibration of a Diatomic Molecule
Approximates an Oscillating Spring

Molecular vibrations

- The positions of atoms in a molecules are not fixed; they are subject to a number of different vibrations.





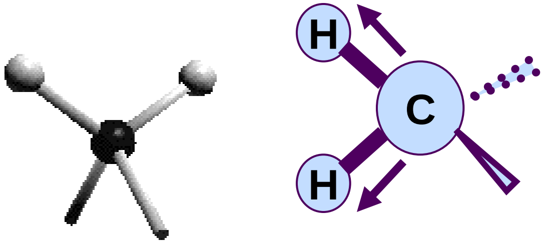
IR Spectroscopy

I. Introduction

C. The IR Spectroscopic Process

5. There are two types of bond vibration:

- ***Stretch*** – Vibration or oscillation along the line of the bond



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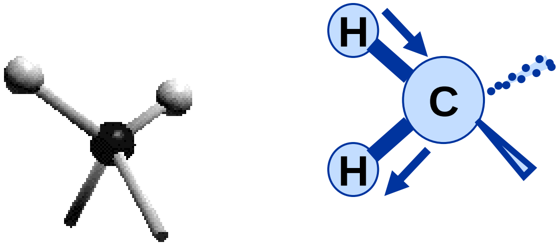
symmetric



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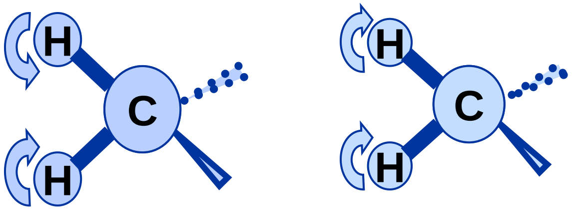
asymmetric

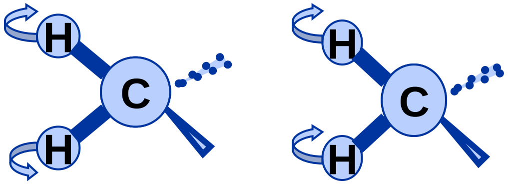
- ***Bend*** – Vibration or oscillation not along the line of the bond



scissor

rock

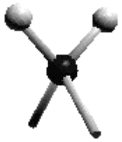
in plane



twist

wag

out of plane



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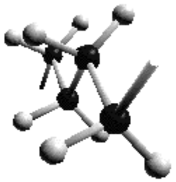

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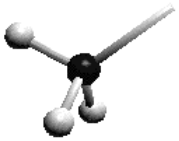

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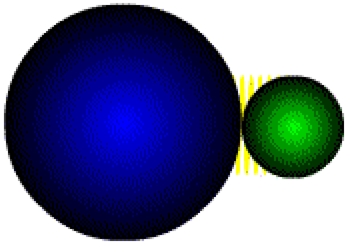
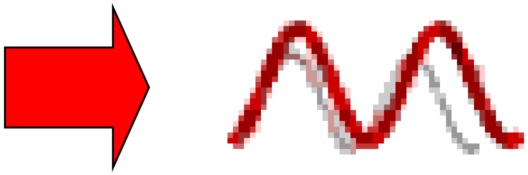
Infrared Spectroscopy

C. The IR Spectroscopic Process

6. As a covalent bond oscillates – due to the oscillation of the dipole of the molecule – a varying electromagnetic field is produced



Vibration of a Diatomic Molecule
Approximates an Oscillating Spring



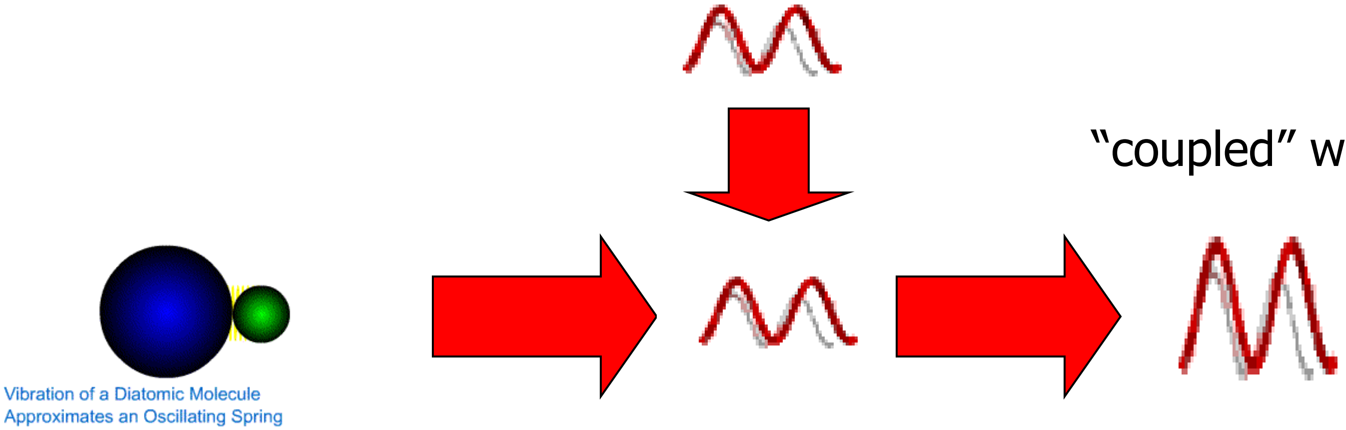
7. The greater the dipole moment change through the vibration, the more intense the EM field that is generated

Infrared Spectroscopy

C. The IR Spectroscopic Process

8. When a wave of infrared light encounters this oscillating EM field generated by the oscillating dipole of the same frequency, the two waves couple, and IR light is absorbed

9. The coupled wave now vibrates with twice the amplitude


Vibration of a Diatomic Molecule Approximates an Oscillating Spring

IR beam from spectrometer

"coupled" wave

EM oscillating wave from bond vibration

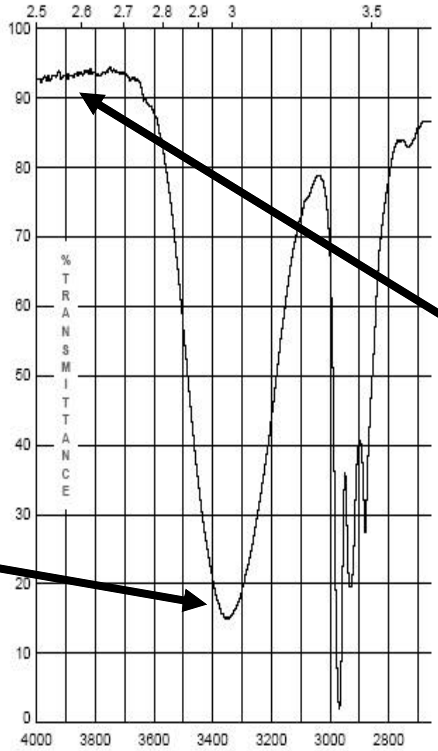
Infrared Spectroscopy

D. The IR Spectrum

1. Each stretching and bending vibration occurs with a characteristic frequency as the atoms and charges involved are different for different bonds

The y-axis on an IR spectrum is in units of % transmittance

In regions where the EM field of an osc. bond interacts with IR light of the same ν – transmittance is low (light is absorbed)

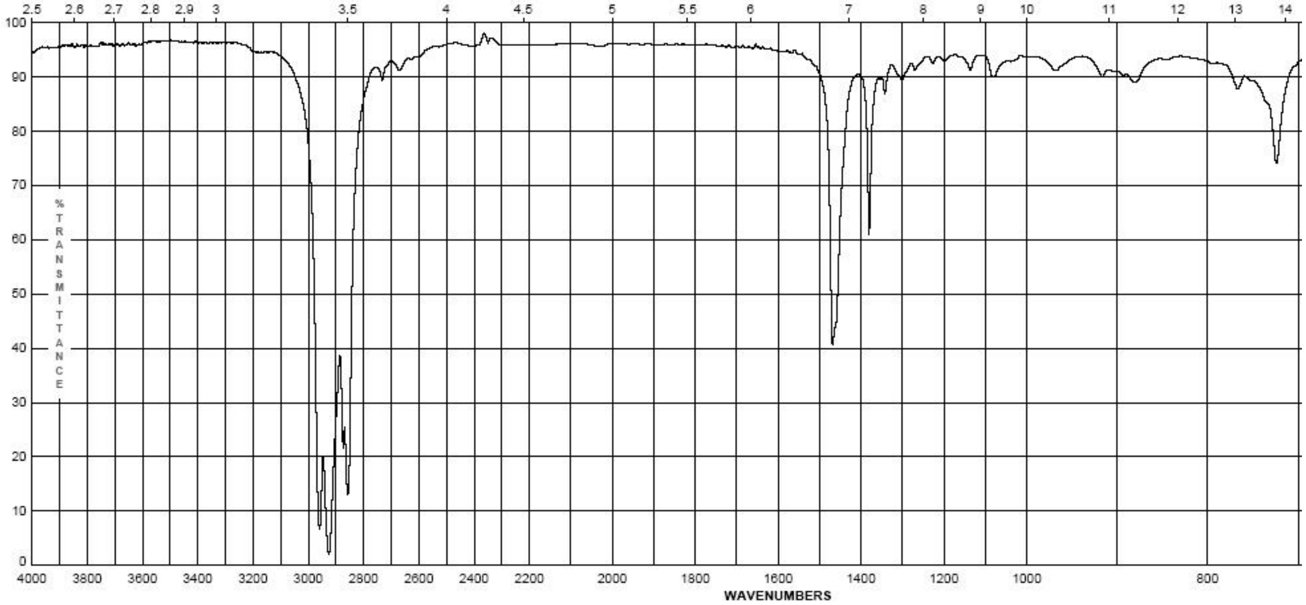


In regions where no osc. bond is interacting with IR light, transmittance nears 100%

IR Spectroscopy

D. The IR Spectrum

2. The x-axis of the IR spectrum is in units of wavenumbers, $\bar{\nu}$, which is the number of waves per centimeter in units of cm^{-1} (Remember $E = h\nu$ or $E = hc/\lambda$)



IR Spectroscopy

D. The IR Spectrum

3. This unit is used rather than wavelength (microns) because wavenumbers are directly proportional to the energy of transition being observed – ***chemists like this, physicists hate it***

   High frequencies and high wavenumbers equate higher energy

   is quicker to understand than

   Short wavelengths equate higher energy

4. This unit is used rather than frequency as the numbers are more "real" than the exponential units of frequency

5. IR spectra are observed for the mid-infrared: 600-4000 cm^{-1}

6. The peaks are Gaussian distributions of the average energy of a transition

IR Spectroscopy

D. The IR Spectrum

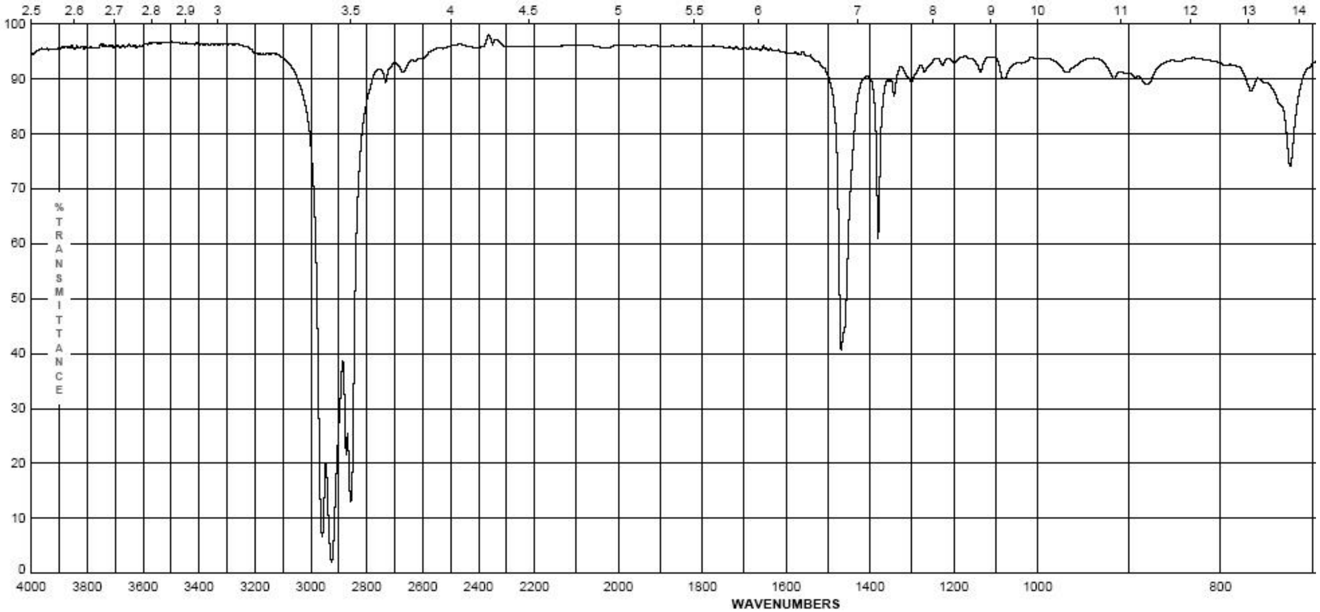
7. In general:

Lighter atoms will allow the oscillation to be faster – *higher energy*

This is especially true of bonds to hydrogen – C-H, N-H and O-H

Stronger bonds will have higher energy oscillations

Triple bonds > double bonds > single bonds in energy



← Energy/ν of oscillation

E. The IR Spectrum – The detection of different bonds

7. As opposed to chromatography or other spectroscopic methods, the area of a IR band (or peak) is not ***directly*** proportional to concentration of the functional group producing the peak

8. The intensity of an IR band is affected by two primary factors:

   Whether the vibration is one of stretching or bending

   Electronegativity difference of the atoms involved in the bond

   - For both effects, the greater the change in dipole moment in a given vibration or bend, the larger the peak.

   - The greater the difference in electronegativity between the atoms involved in bonding, the larger the dipole moment

   - Typically, stretching will change dipole moment more than bending

E. The IR Spectrum – The detection of different bonds

9. It is important to make note of peak intensities to show the effect of these factors:

- ***Strong (s)*** – peak is tall, transmittance is low (0-35 %)
- ***Medium (m)*** – peak is mid-height (75-35%)
- ***Weak* (w)** – peak is short, transmittance is high (90-75%)
- **** Broad (br)*** – if the Gaussian distribution is abnormally broad *(*this is more for describing a bond that spans many energies)*

Exact transmittance values are rarely recorded

II. Infrared Group Analysis

A. General

1. The primary use of the IR is to ***detect functional groups***

2. Because the IR looks at the interaction of the EM spectrum with actual bonds, it provides a unique qualitative probe into the functionality of a molecule, as functional groups are merely different configurations of different types of bonds

3. Since most “types” of bonds in covalent molecules have roughly the same energy, i.e., C=C and C=O bonds, C-H and N-H bonds they show up in similar regions of the IR spectrum

4. Remember all organic functional groups are made of multiple bonds and therefore show up as multiple IR bands (peaks)

Infrared Spectroscopy

Region of infrared that is most useful lies between
2.5-16 *m*m (4000-625 cm^{-1})

depends on transitions between vibrational
energy states

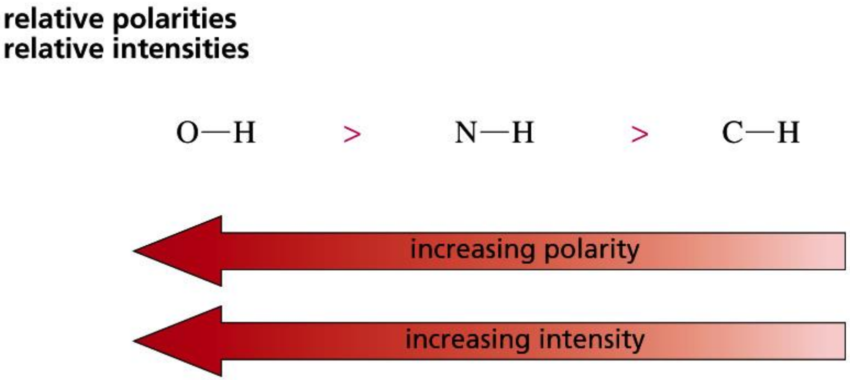
Stretching: higher energy / higher wave number (cm^{-1})

Bending: lower energy / lower wave number (cm^{-1})

A bond must have a dipole or an induced dipole in order to have an absorbance in the IR spectrum.

When the bond stretches, the increasing distance between the atoms increases the dipole moment.

Therefore, the greater the dipole, the more intense the absorption. (i.e., The greater the molar extinction coefficient (ε) in Beer's law, $A = \varepsilon bc$.



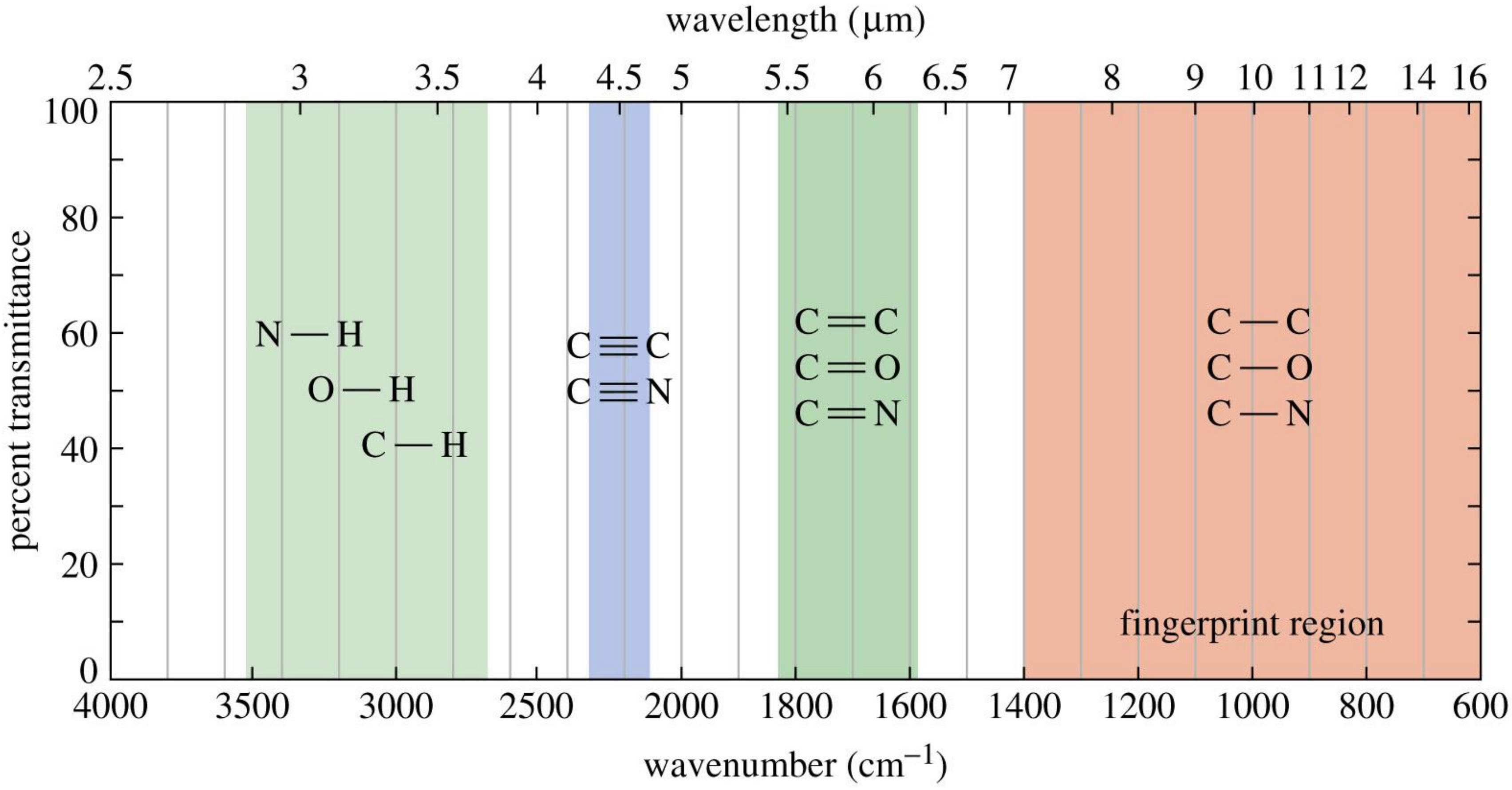
Analyzing Structure: Functions & Infrared Spectra

The molecular formula is a critical piece of information, which limits the functional possibilities.

The presence & absence of absorption bands must be considered in identifying a possible structure in IR spectroscopy. Empiricism is critical to successful identification.

NOTE: Bonds which lack dipole moments are not detected.

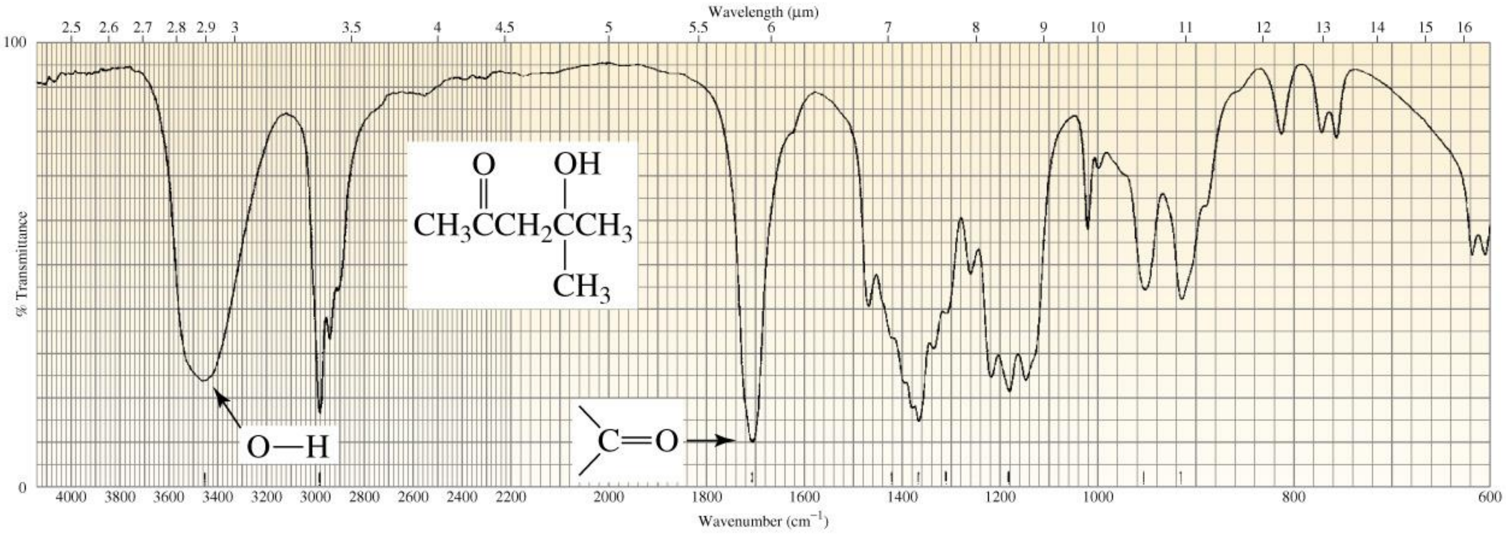
Structural/Functional Components



Important IR Stretching Frequencies

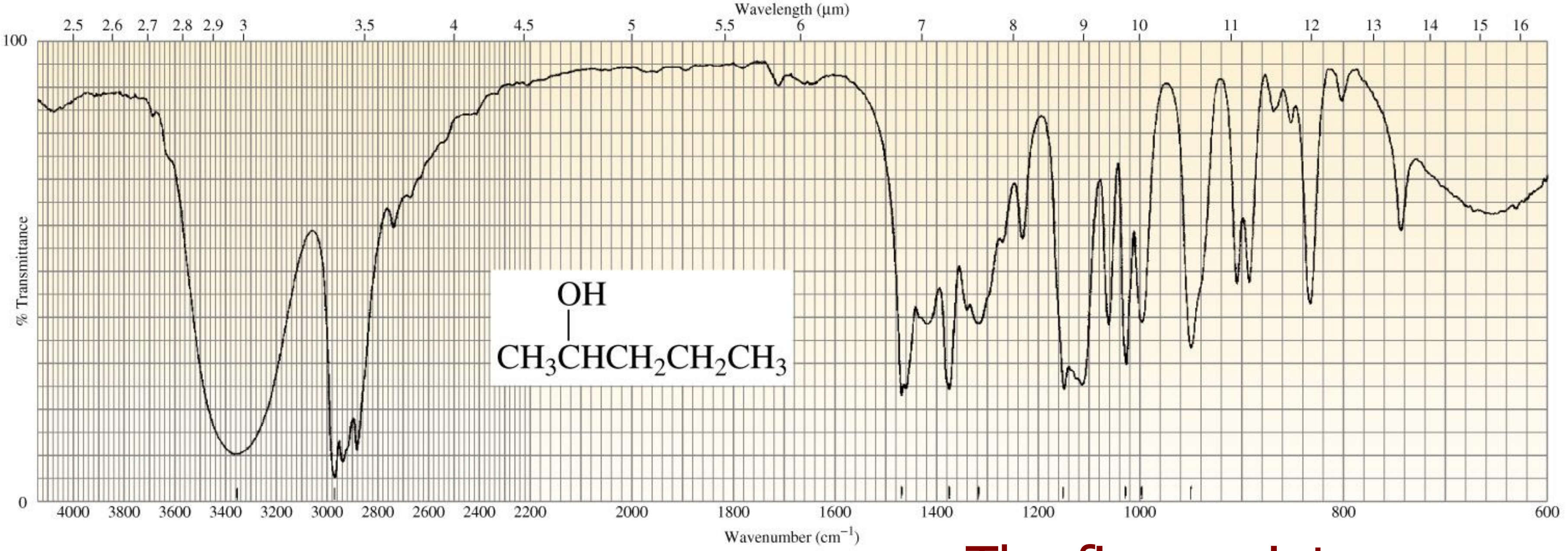
Type of bond	Wavenumber (cm^{-1})	Intensity
$C\equiv N$	2260–2220	medium
$C\equiv C$	2260–2100	medium to weak
$C=C$	1680–1600	medium
$C=N$	1650–1550	medium
	~1600 and ~1500–1430	strong to weak
$C=O$	1780–1650	strong
$C-O$	1250–1050	strong
$C-N$	1230–1020	medium
$O-H$ (alcohol)	3650–3200	strong, broad
$O-H$ (carboxylic acid)	3300–2500	strong, very broad
$N-H$	3500–3300	medium, broad
$C-H$	3300–2700	medium

An Infrared Spectrum



The peaks are quantized absorption bands corresponding to molecular stretching and bending vibrations

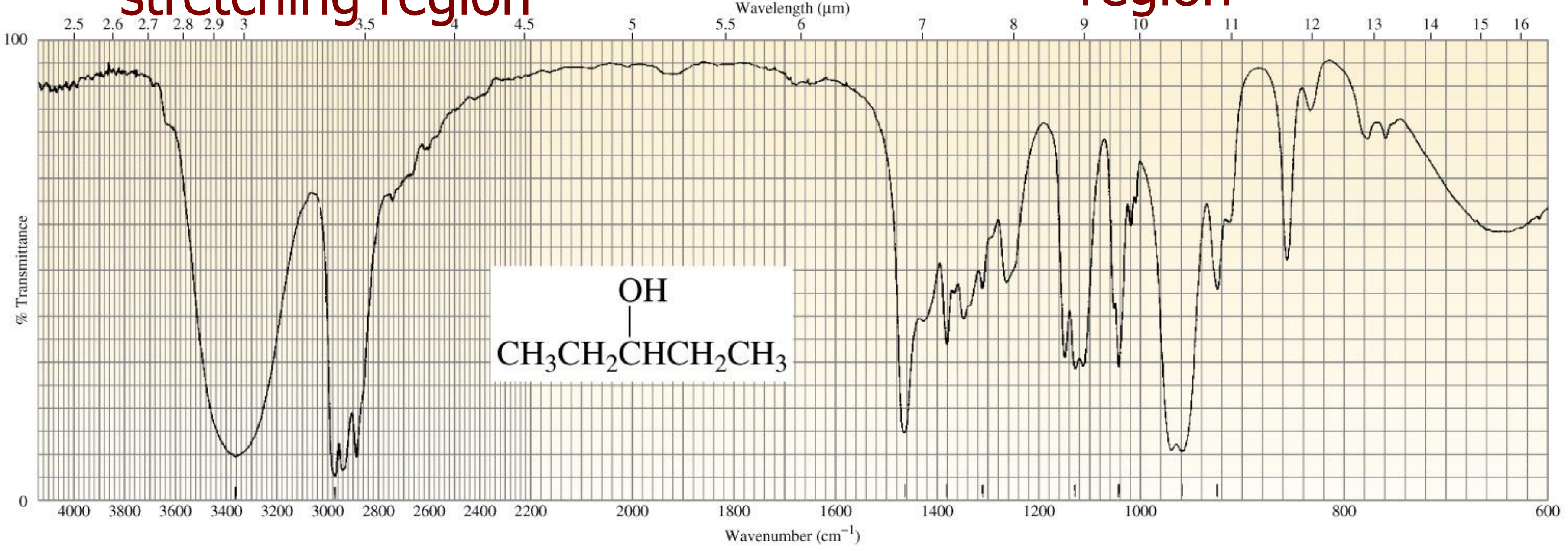
a.



The functional group stretching region

The fingerprint region

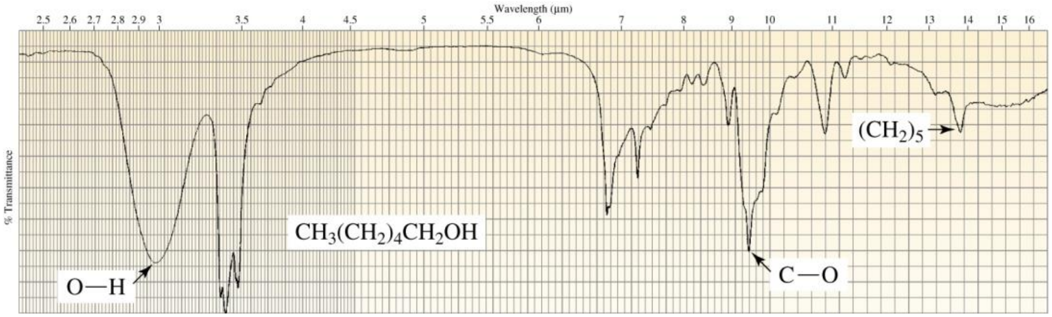
b.

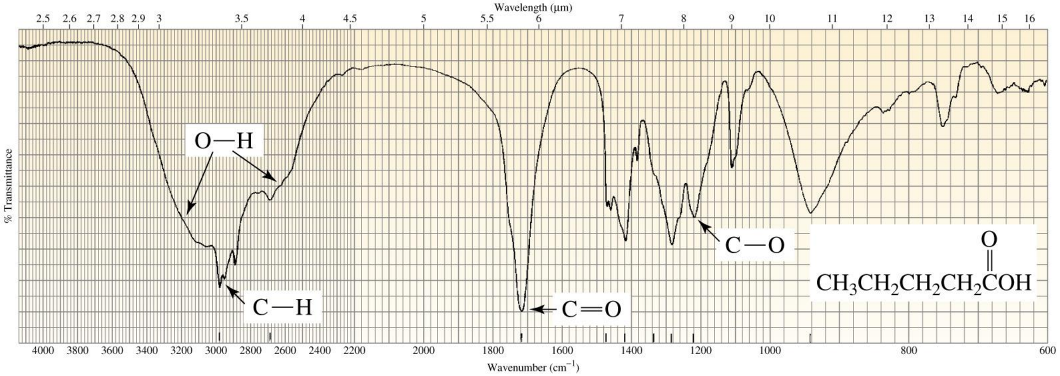


Infrared Absorption Frequencies

Structural unit	Frequency, cm^{-1}
Stretching vibrations (single bonds)	
O—H (alcohols)	3200-3600
O—H (carboxylic acids)	3000-3100

First examine the absorption bands in the vicinity of 4000-3000 cm^{-1}


Wavelength (μm)
2.5 2.6 2.7 2.8 2.9 3 3.5 4 4.5 5 5.5 6 7 8 9 10 11 12 13 14 15 16
% Transmittance
$CH_3(CH_2)_4CH_2OH$
O—H
C—O
$(CH_2)_5$

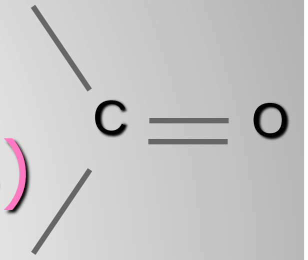

Wavelength (μm)
2.5 2.6 2.7 2.8 2.9 3 3.5 4 4.5 5 5.5 6 7 8 9 10 11 12 13 14 15 16
% Transmittance
O—H
C—H
C=O
C—O
$CH_3CH_2CH_2CH_2\overset{O}{\overset{\|}{C}}OH$
4000 3800 3600 3400 3200 3000 2800 2600 2400 2200 2000 1800 1600 1400 1200 1000 800 600
Wavenumber (cm^{-1})

Infrared Absorption Frequencies

Structural unit	Frequency, cm^{-1}
Stretching vibrations (single bonds)	
sp C—H	3310-3320
sp^2 C—H	3000-3100
sp^3 C—H	2850-2950
sp^2 C—O	1200
sp^3 C—O	1025-1200

Infrared Absorption Frequencies

Structural unit	Frequency, cm^{-1}



Stretching vibrations (carbonyl groups)

Aldehydes and ketones 1710-1750

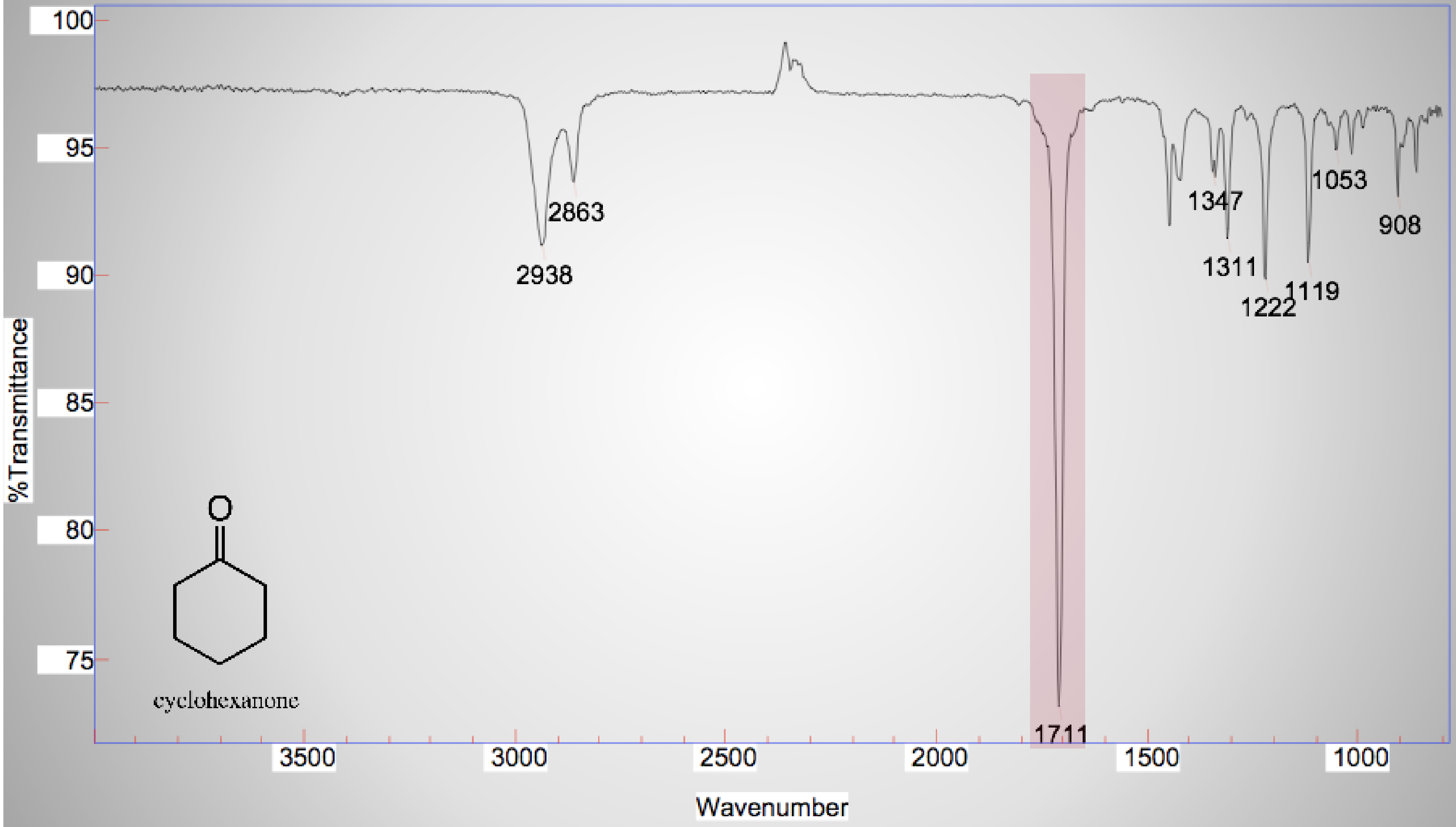
Carboxylic acids: 1700-1725

Acid anhydrides: 1800-1850 and 1740-1790

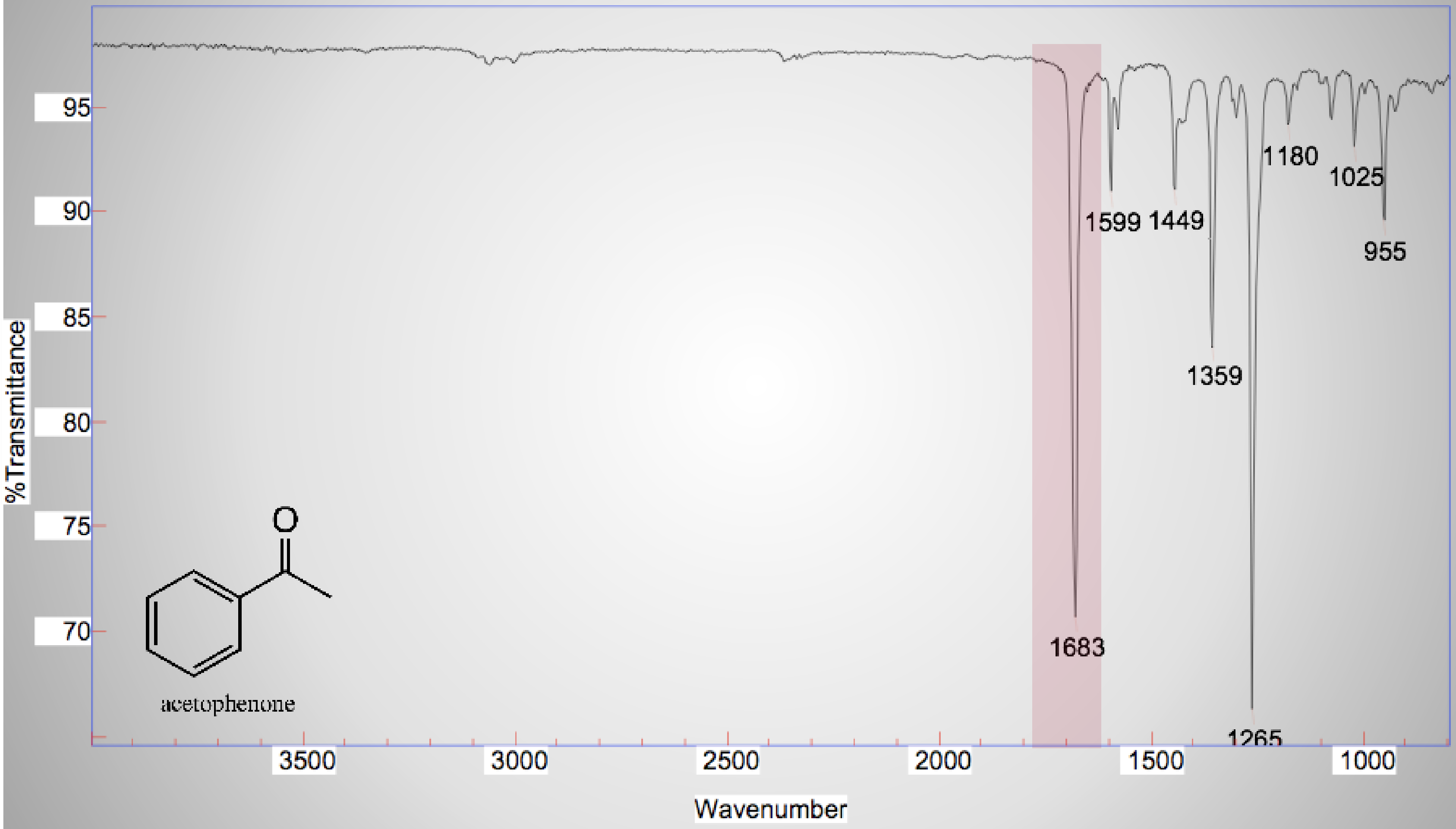
Esters: 1730-1750

Amides: 1680-1700

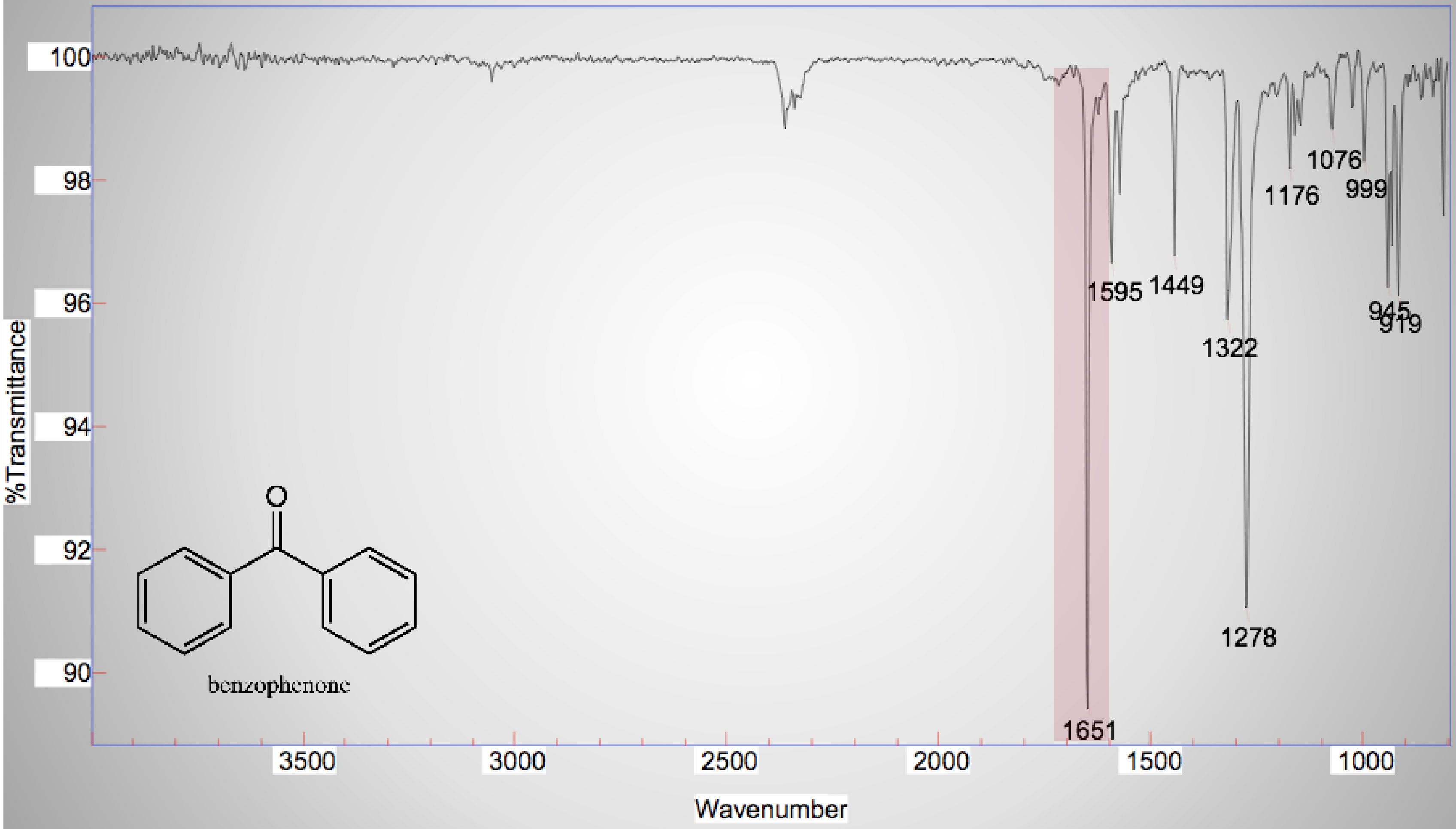
Cyclic aliphatic ketone



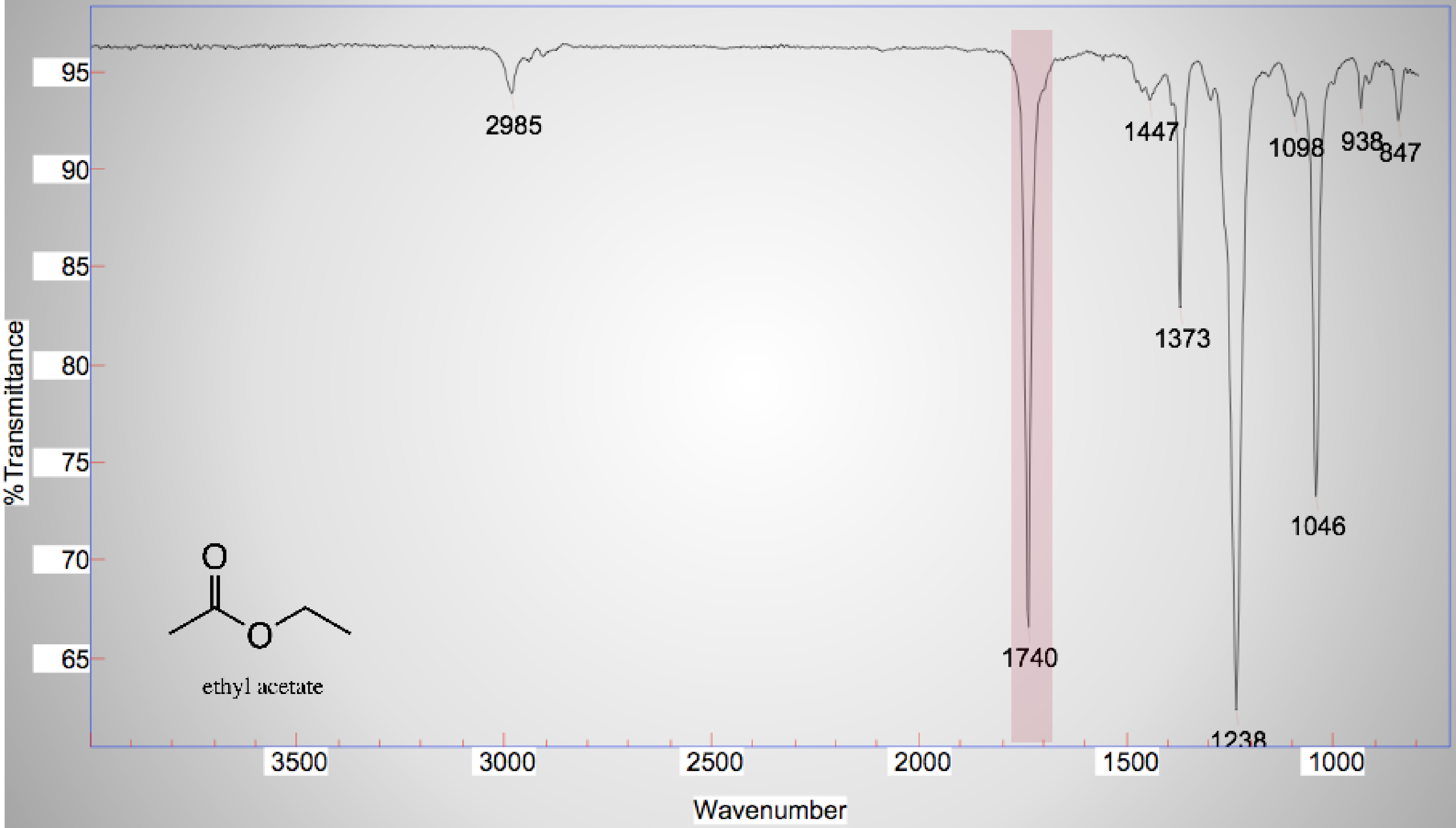
Mono substituted aromatic methyl ketone



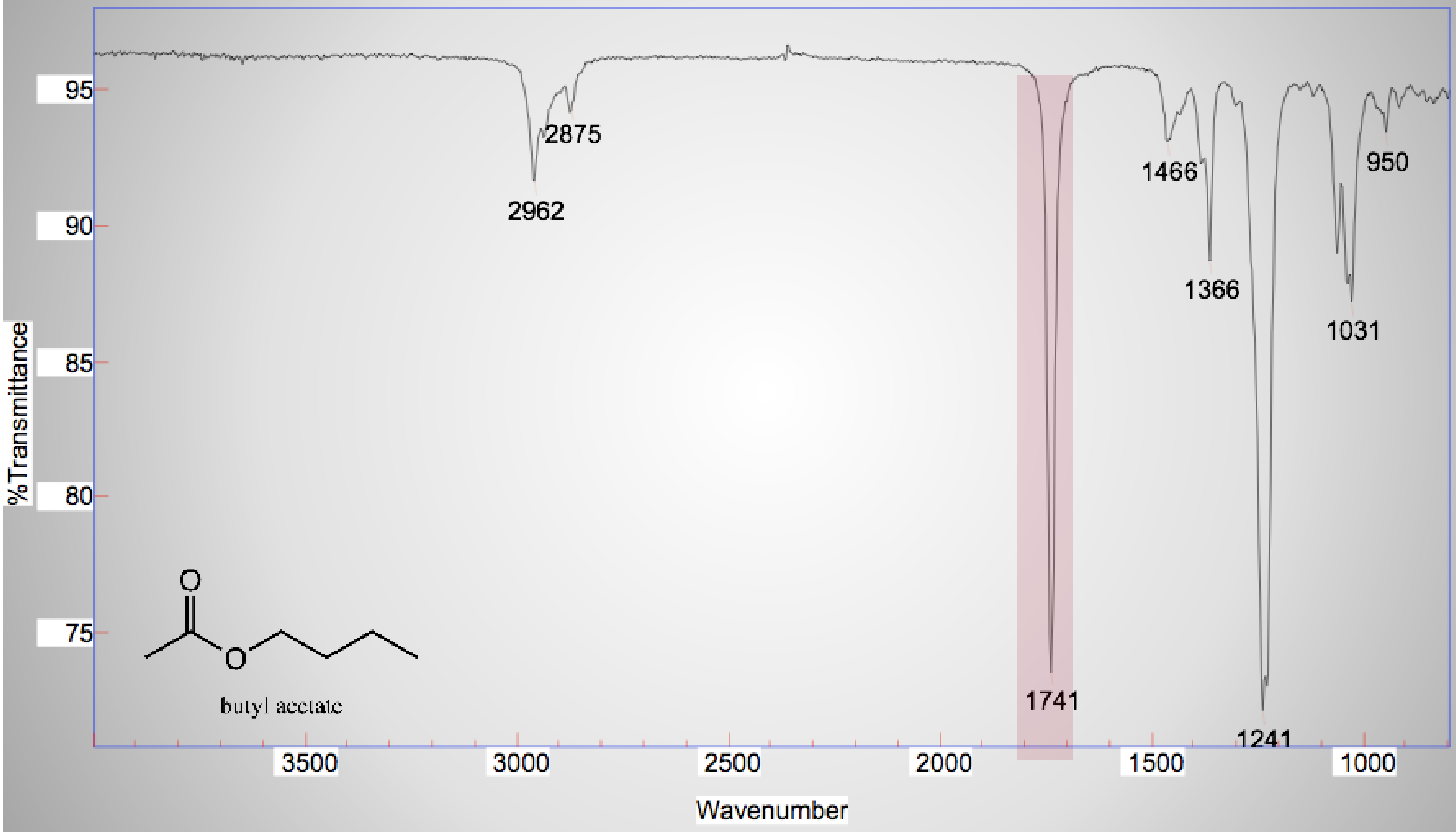
Mono substituted aromatic ketone



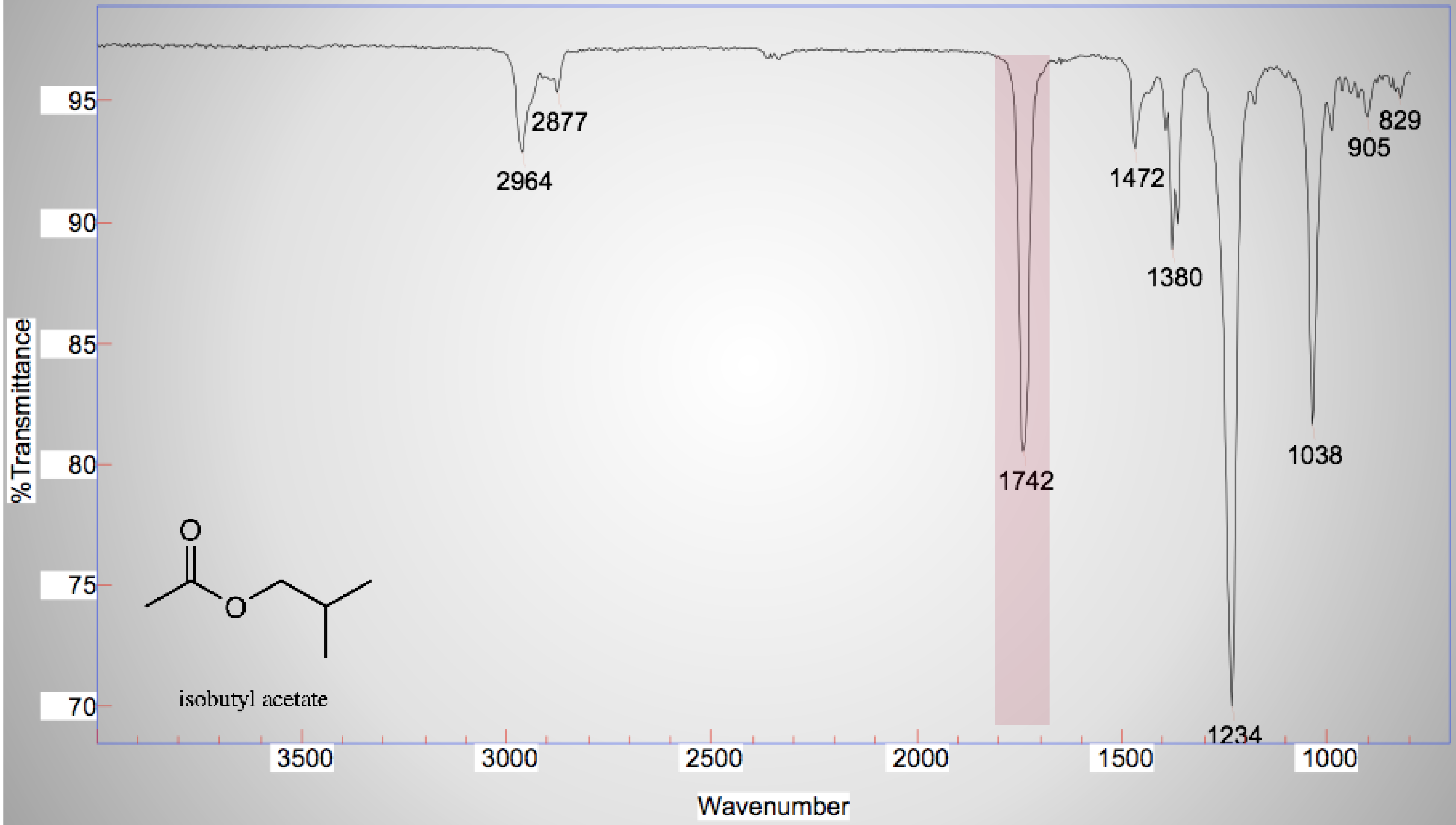
Aliphatic ester I



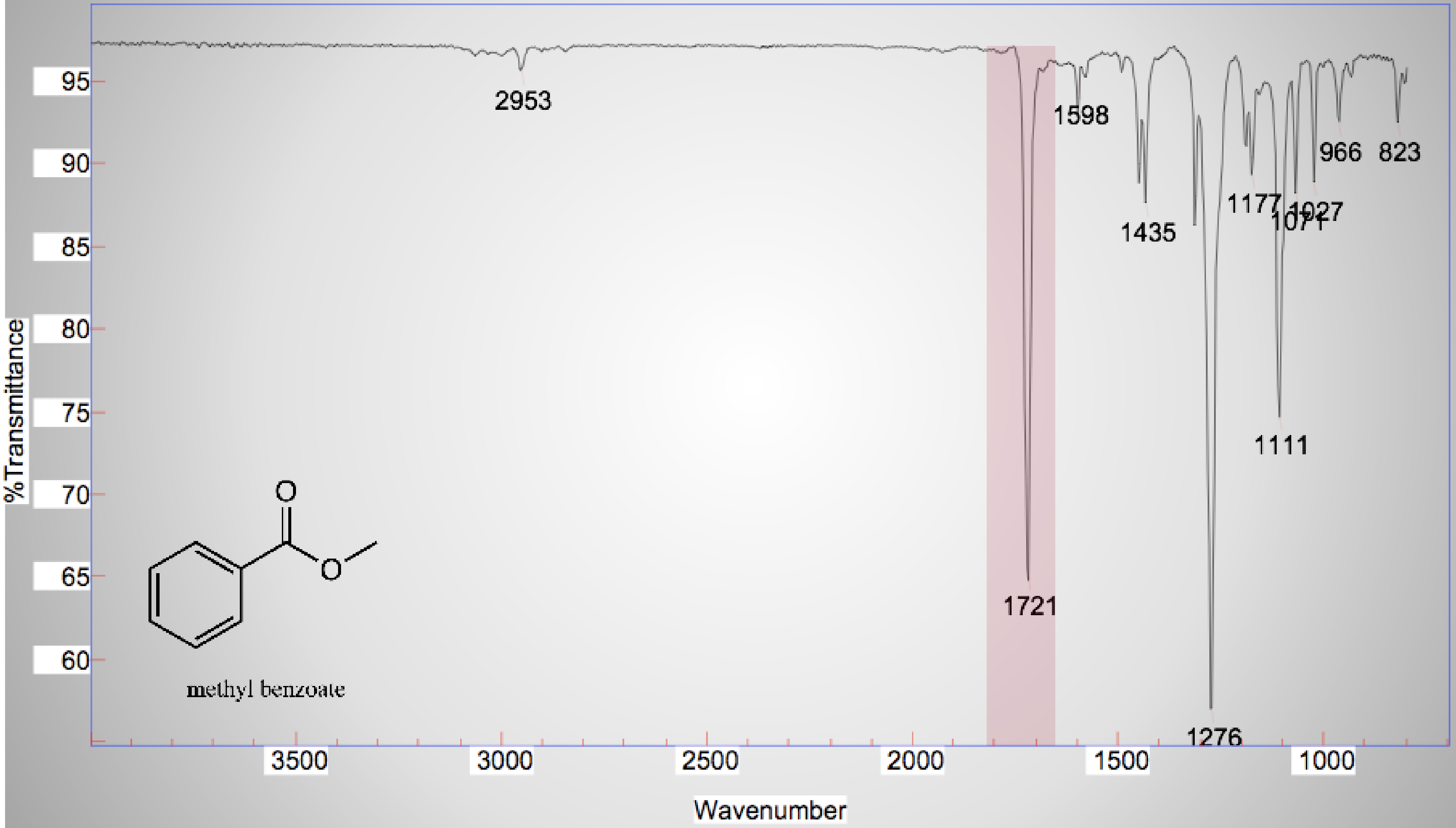
Aliphatic ester II



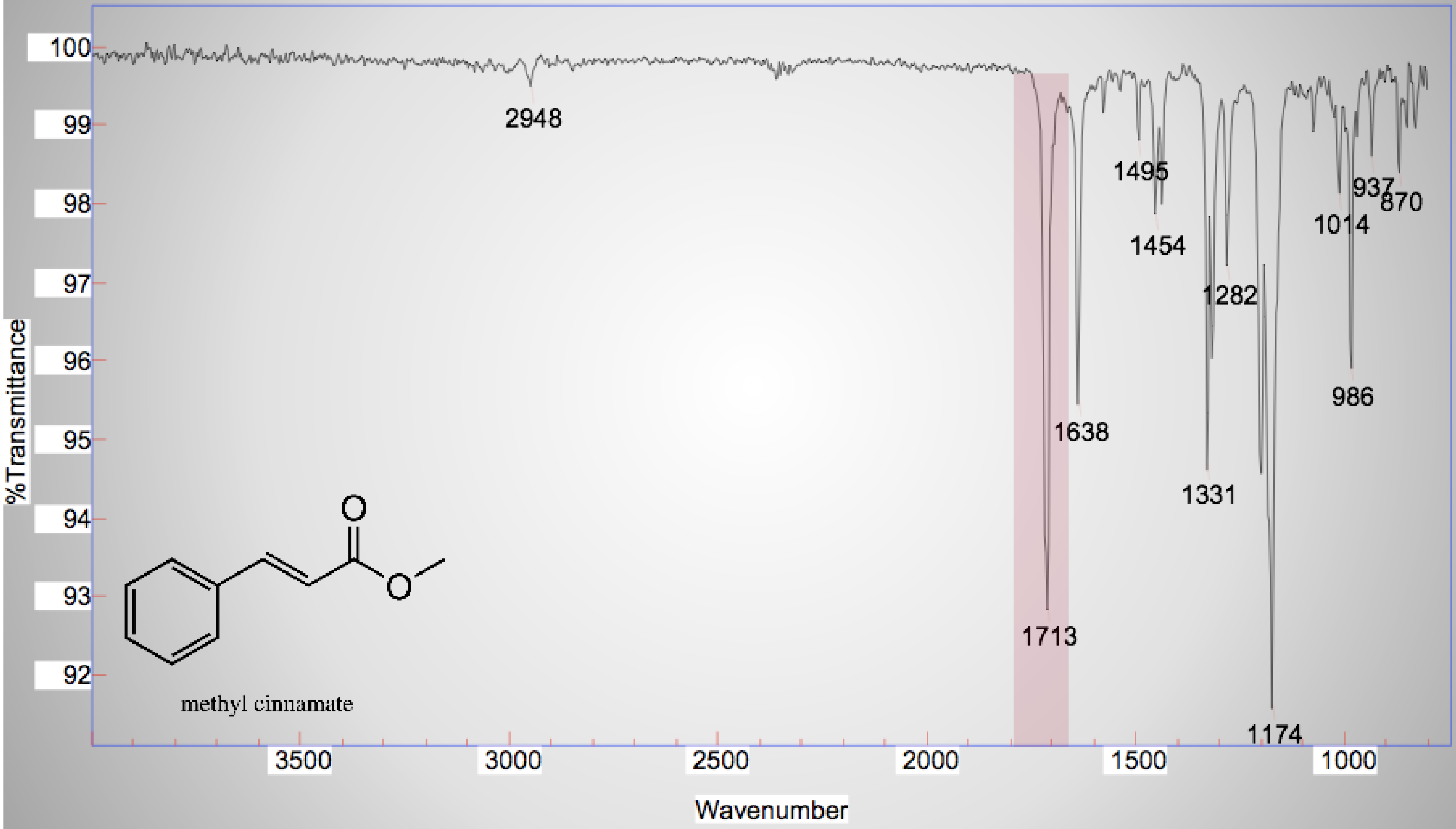
Aliphatic ester III



Mono substituted aromatic ester



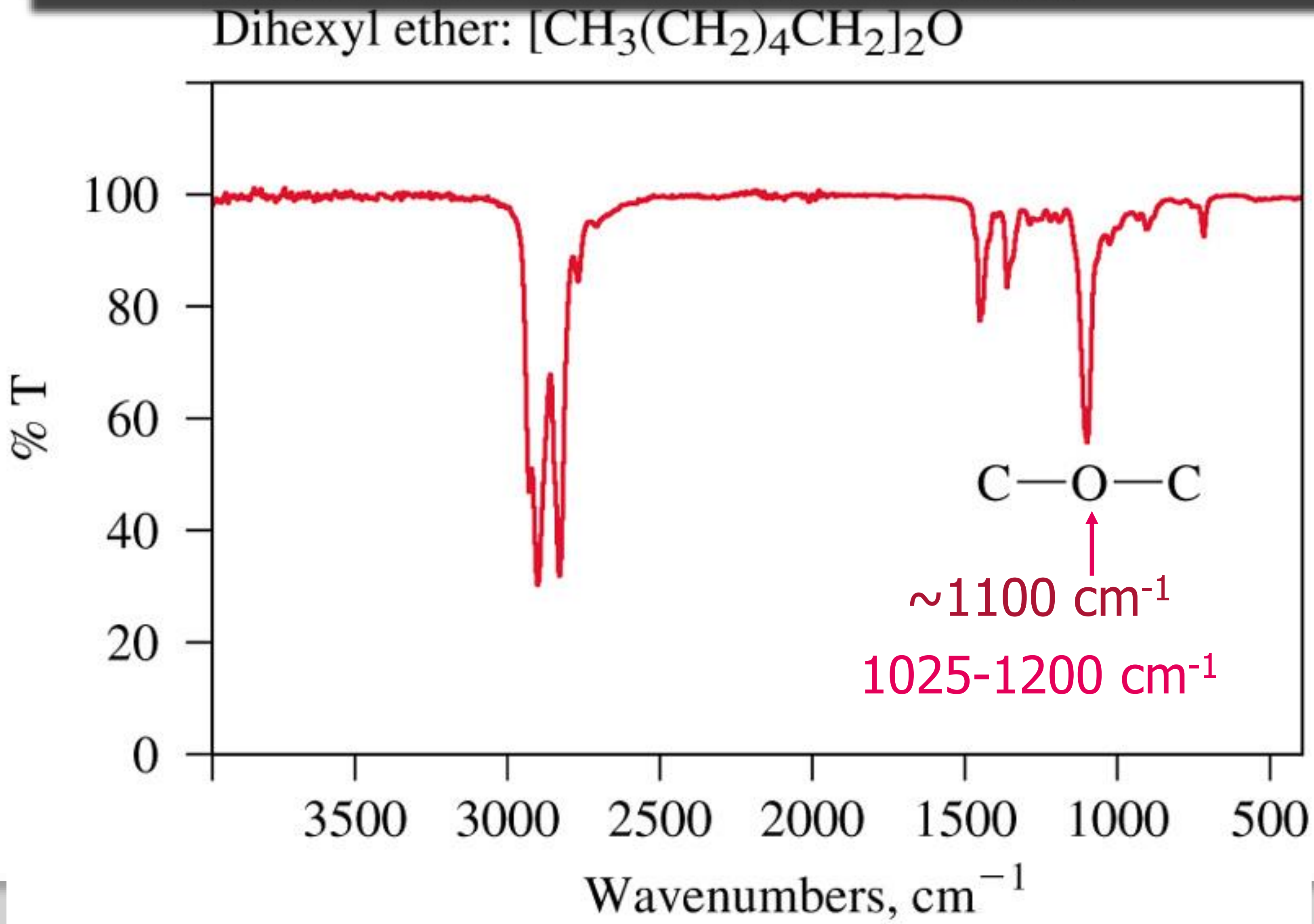
Mono substituted aromatic conjugated ester



Infrared Absorption Frequencies

Structural unit	Frequency, cm^{-1}
Stretching vibrations (single bonds)	
sp^2 C—O	1200
sp^3 C—O	1025-1200

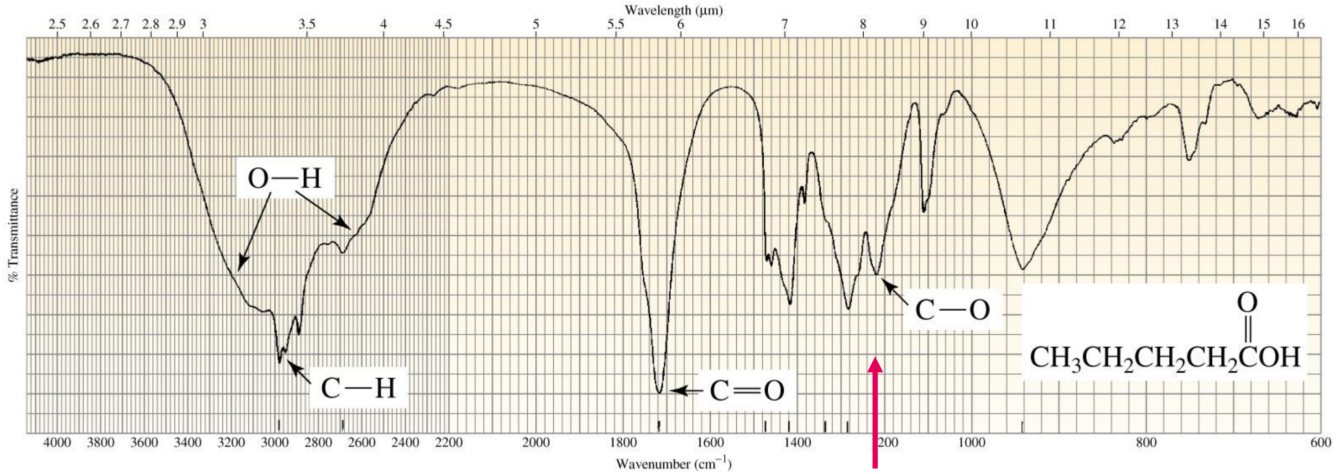
Dihexyl Ether



~1100 cm^{-1}

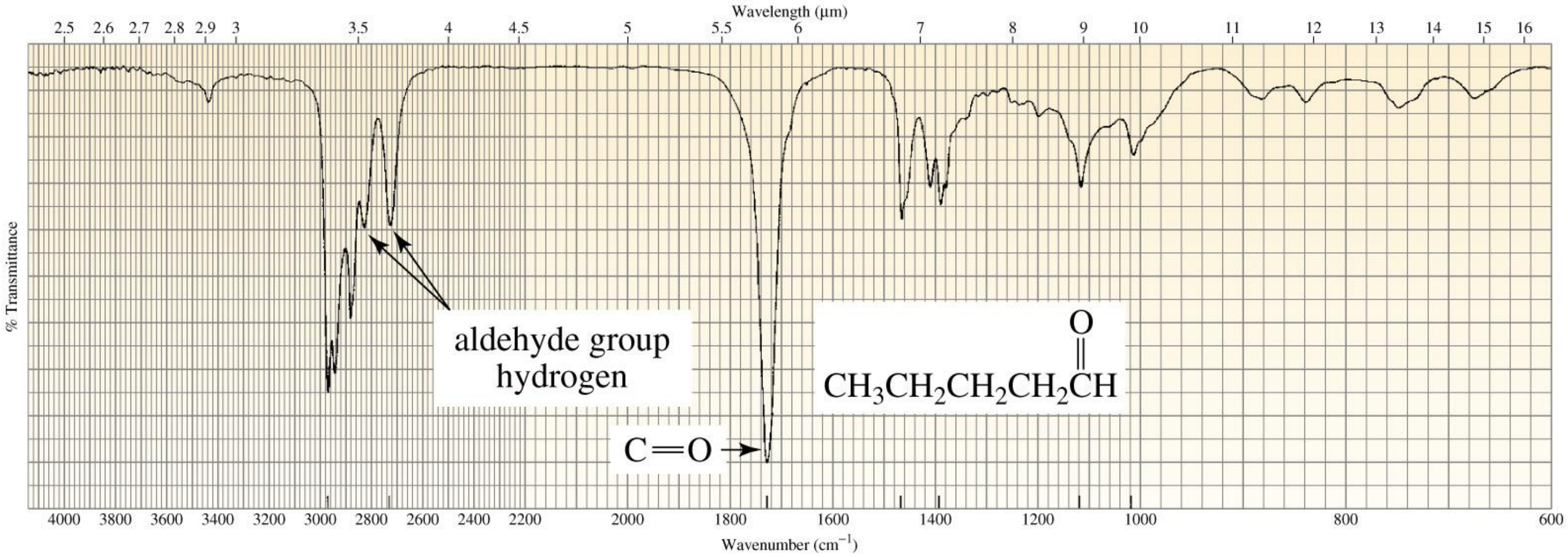
1025-1200 cm^{-1}

Carboxylic Acid

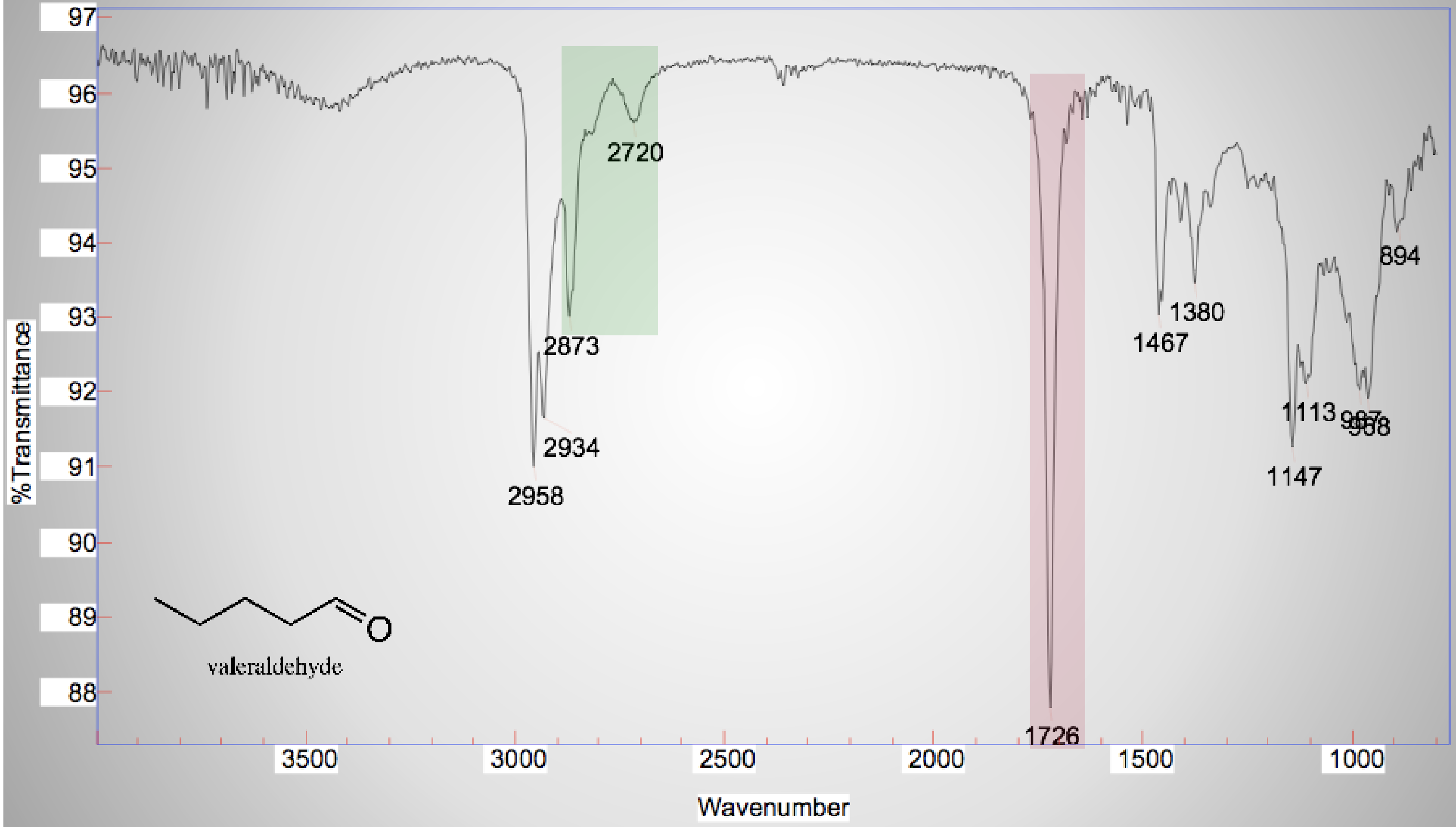


~1200 cm^{-1}

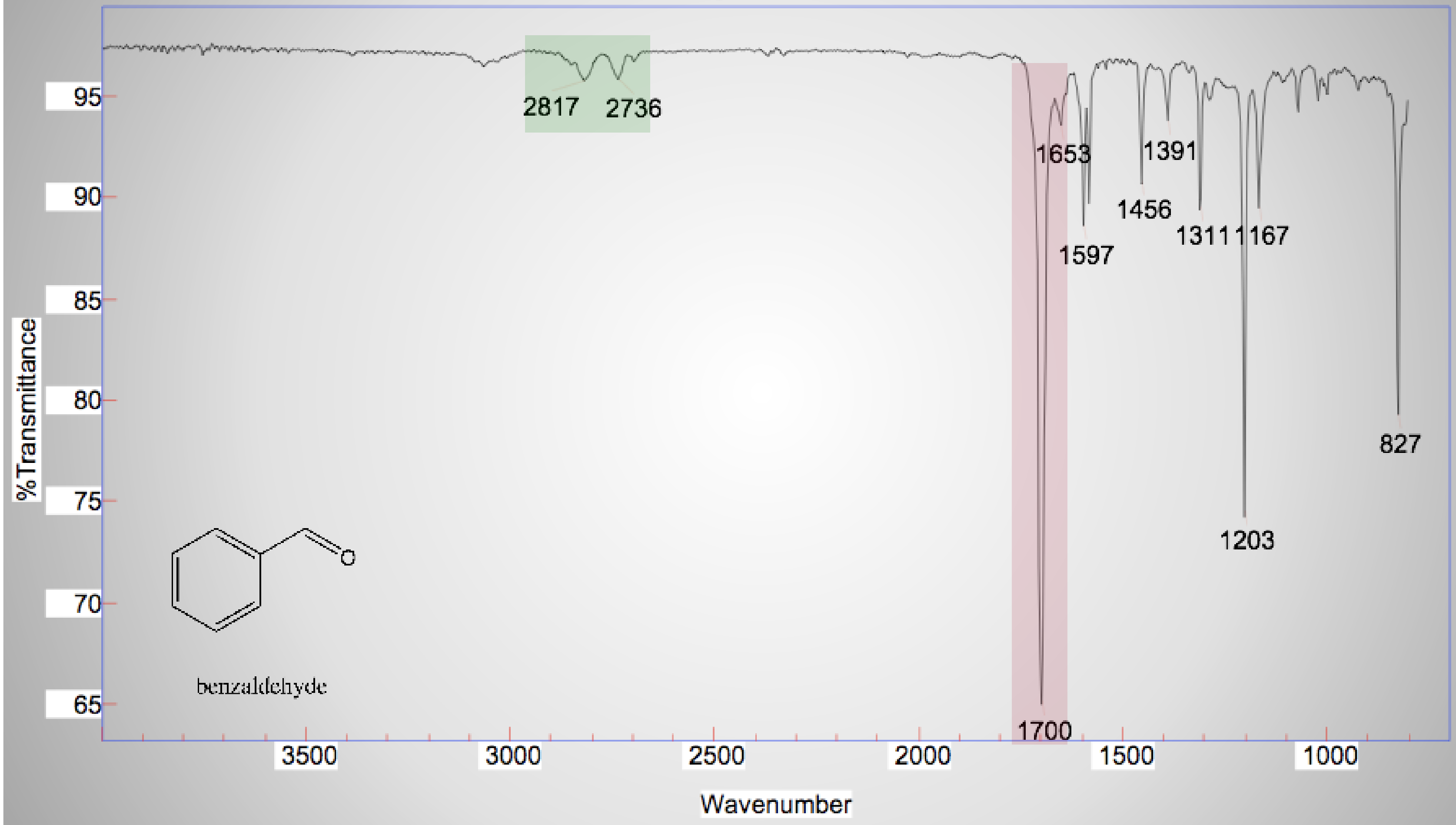
Distinctive Stretch of C–H Bond in an Aldehyde (the "waggle" vibration)



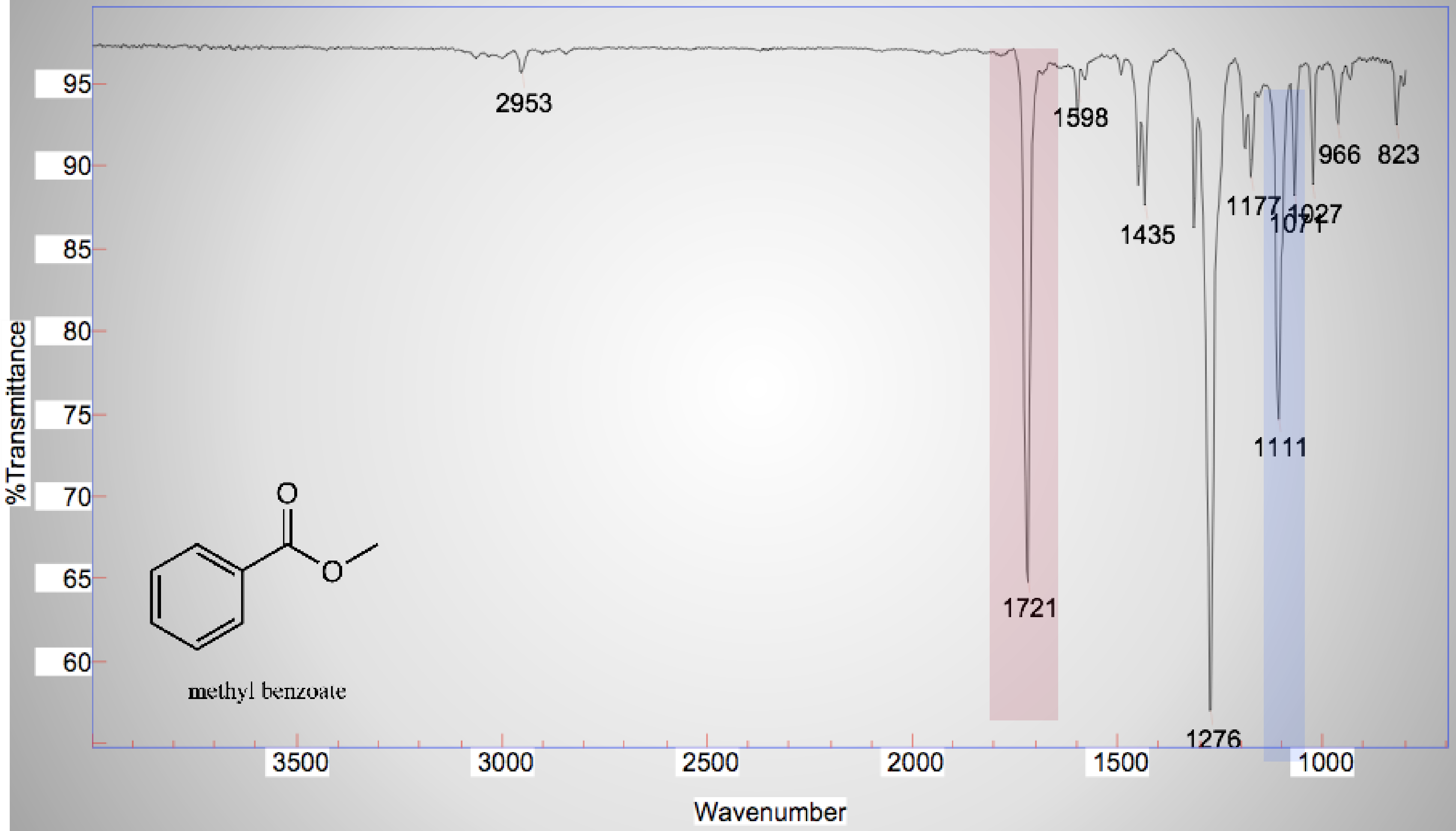
Aliphatic aldehyde



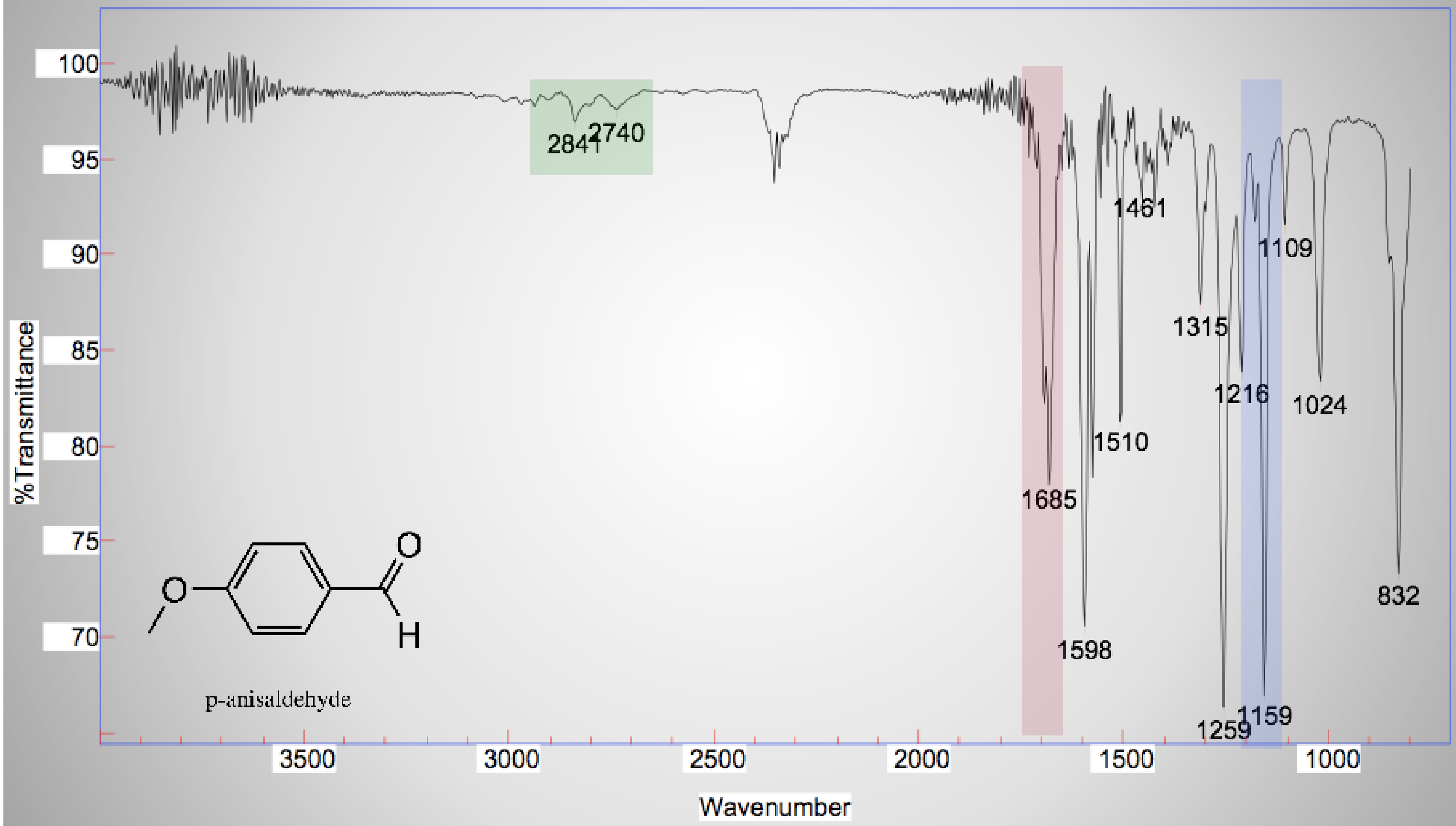
Mono-substituted aromatic aldehyde



Mono substituted aromatic ester



Para di-substituted aromatic ether & aldehyde

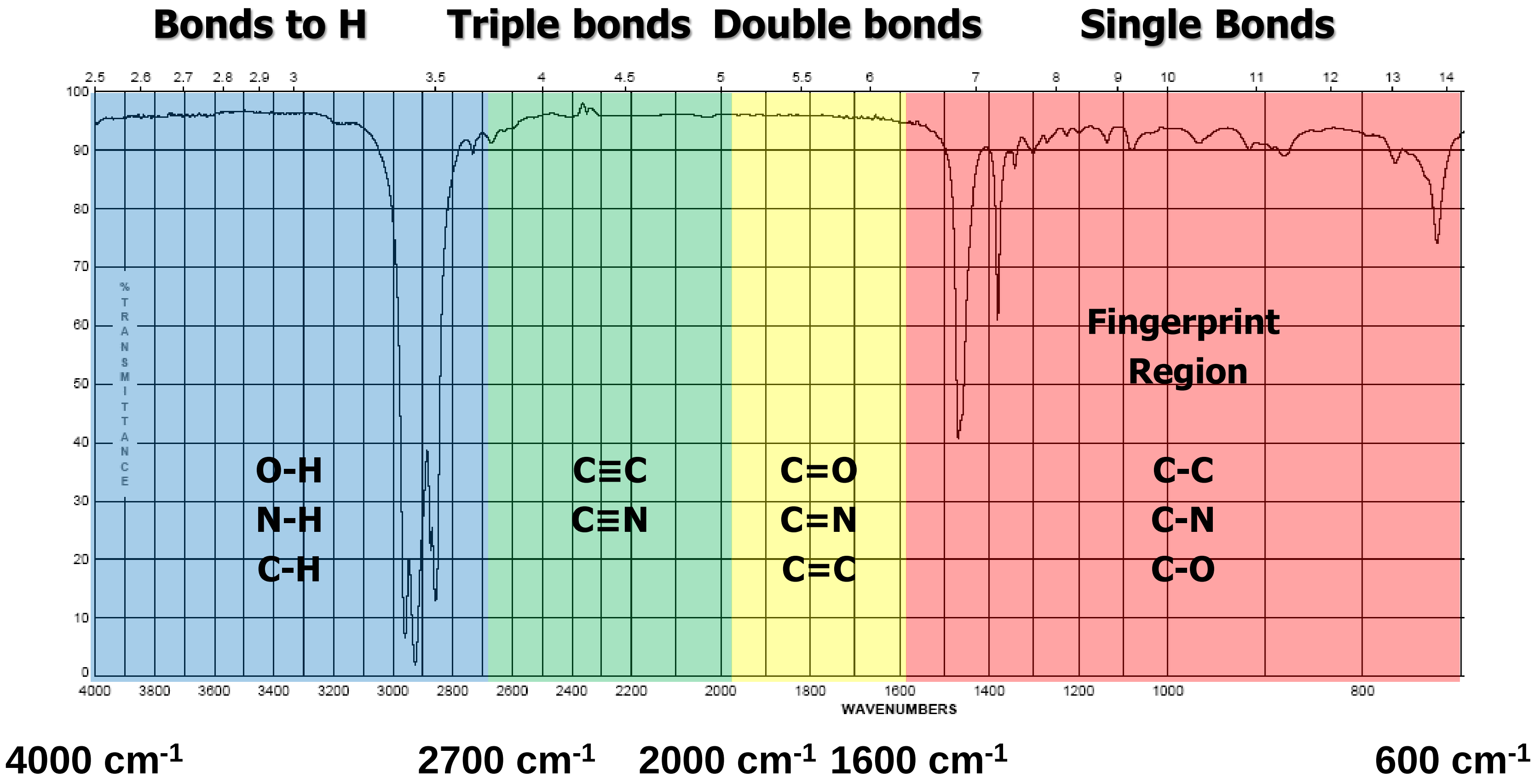


Infrared Spectroscopy

II. Infrared Group Analysis

A. General

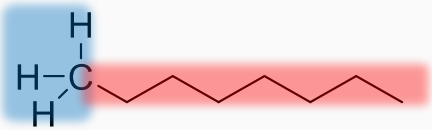
5. The four primary regions of the IR spectrum

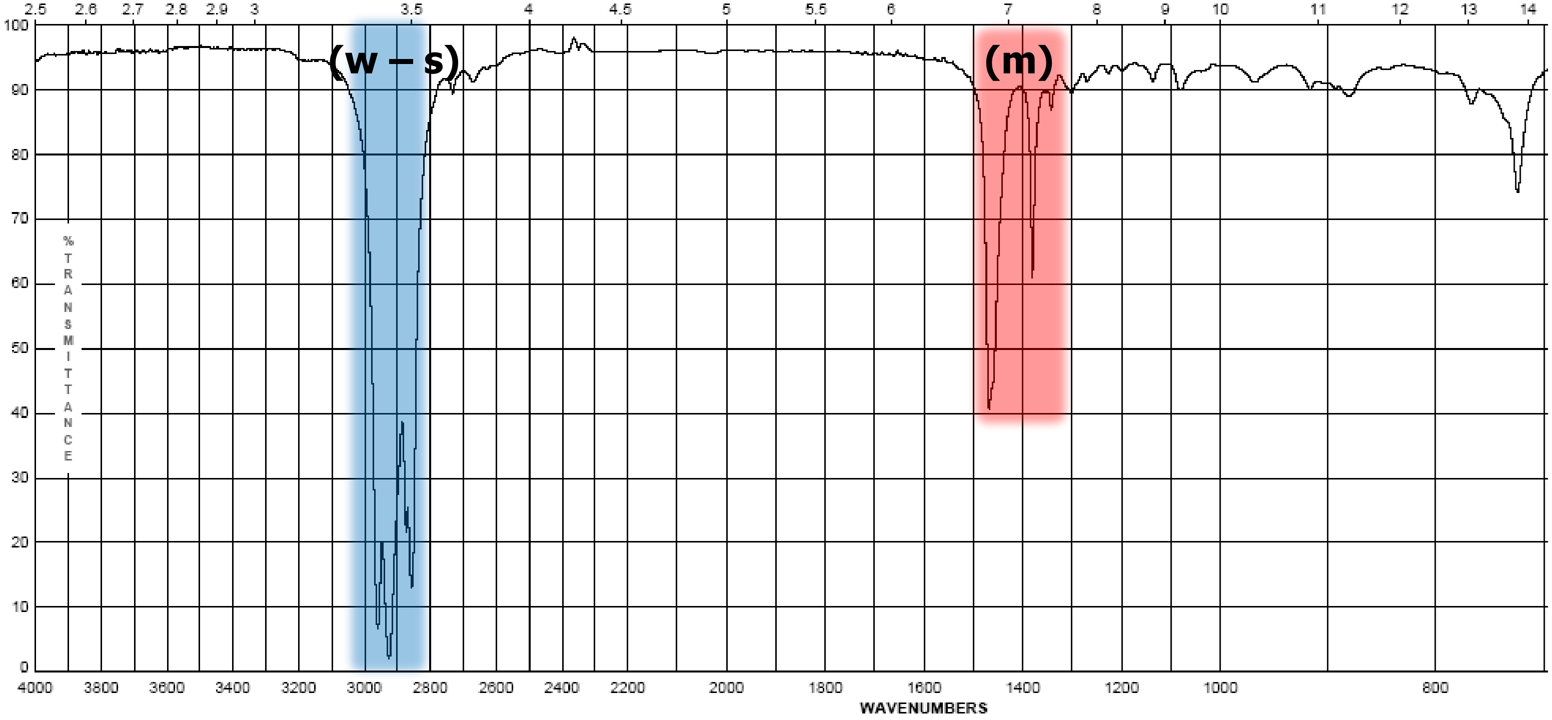


Infrared Spectroscopy

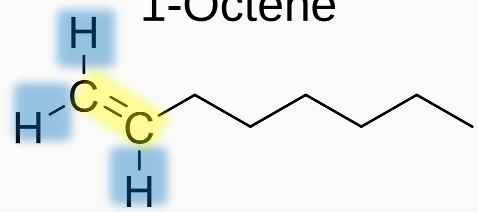
1. **Alkanes** – combination of C-C and C-H bonds
   - C-C stretches and bends 1360-1470 cm^{-1}
   - CH_2-CH_2 bond 1450-1470 cm^{-1}
   - CH_2-CH_3 bond 1360-1390 cm^{-1}
   - sp^3 C-H between 2800-3000 cm^{-1}

Octane



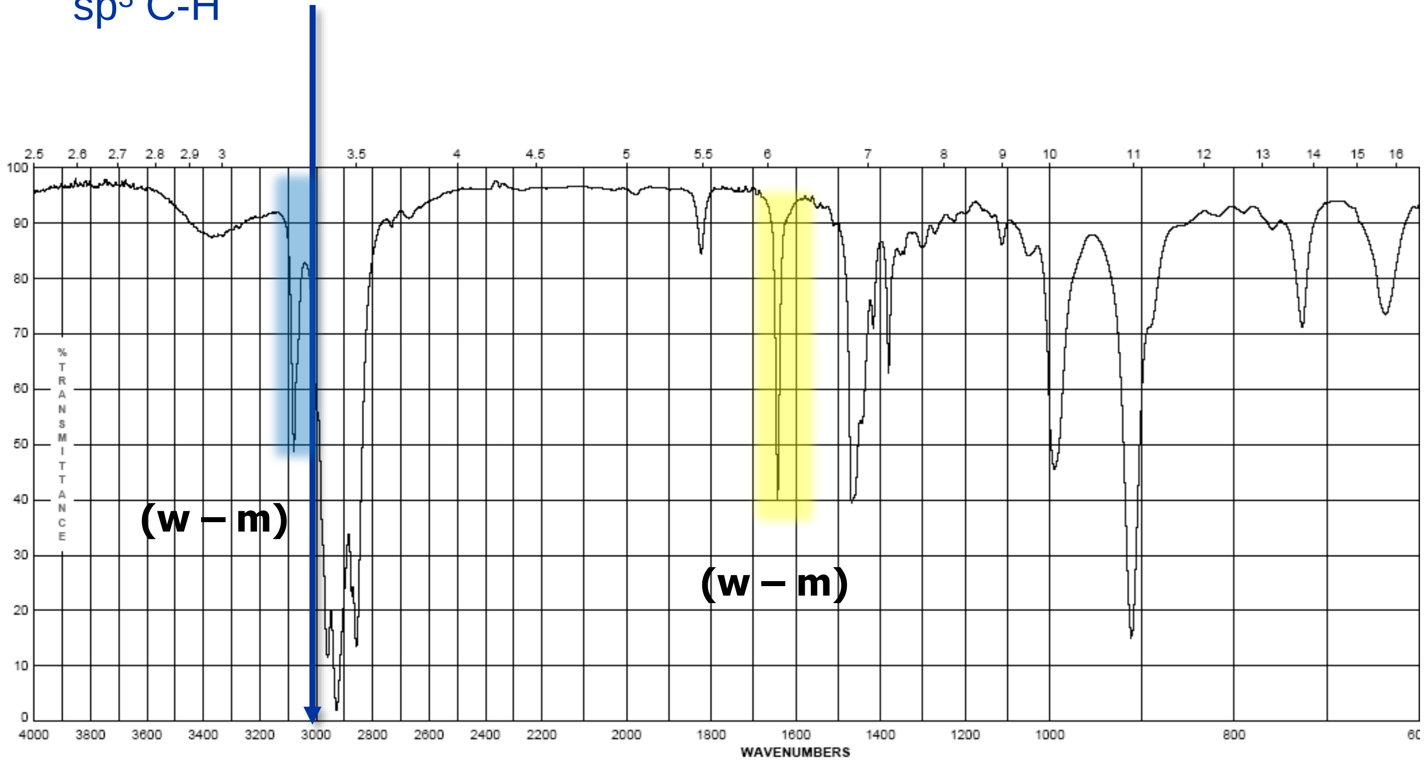


Infrared Spectroscopy



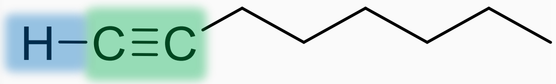
1-Octene

2. **Alkenes** – addition of the C=C and vinyl C-H bonds
   - C=C stretch at 1620-1680 cm^{-1} weaker as substitution increases
   - vinyl C-H stretch occurs at 3000-3100 cm^{-1}
   - The difference between alkane, alkene or alkyne C-H is important! If the band is slightly above 3000 it is vinyl sp^2 C-H or alkynyl sp C-H if it is below it is alkyl sp^3 C-H



Infrared Spectroscopy

1-Octyne

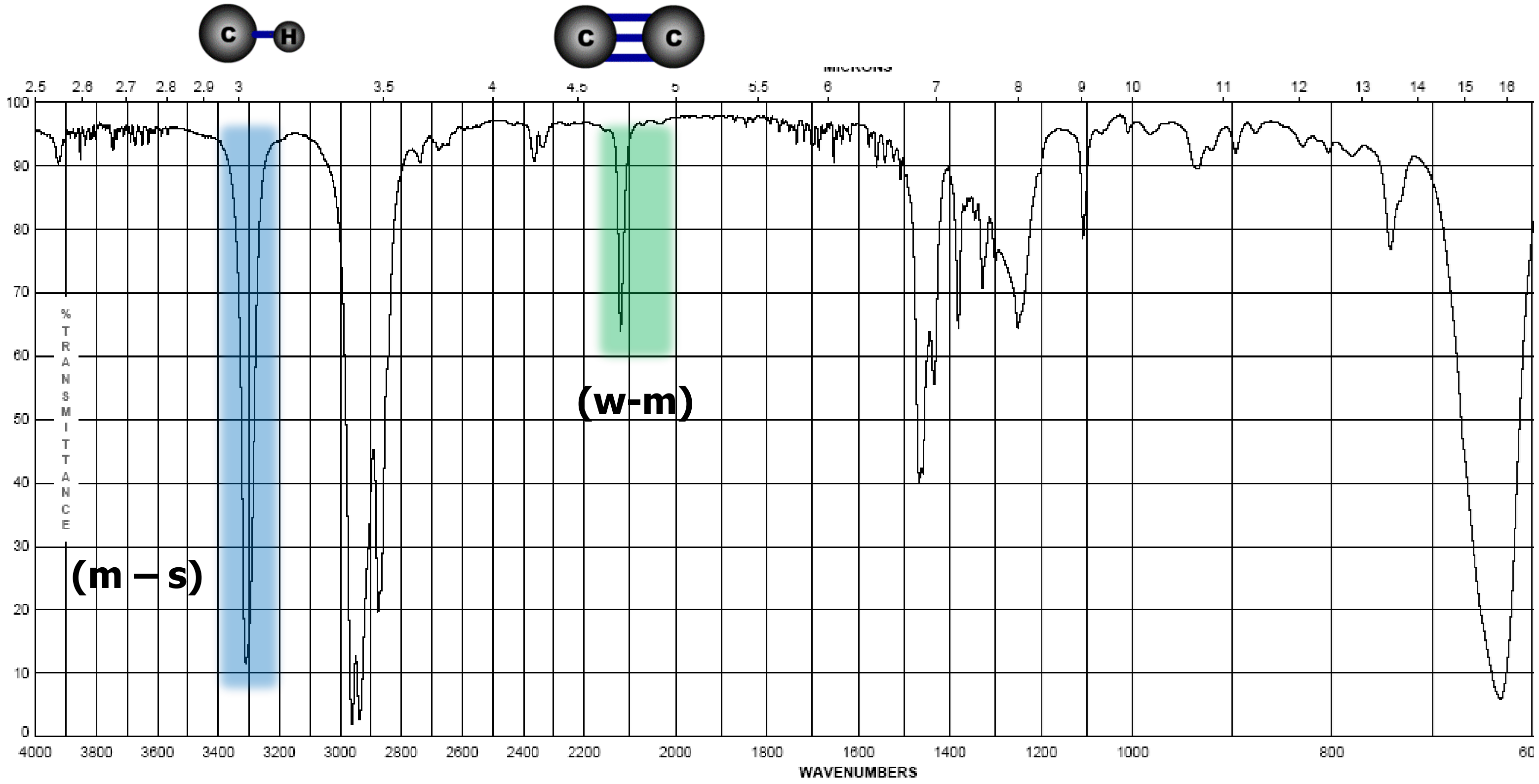


3. **Alkynes** – addition of the C=C and vinyl C-H bonds

- C≡C stretch 2100-2260 cm^{-1}; strength depends on asymmetry of bond, strongest for terminal alkynes, weakest for symmetrical internal alkynes

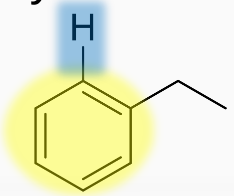
- C-H for ***terminal*** alkynes occurs at 3200-3300 cm^{-1}

- Internal alkynes (R-C≡C-R) would not have this band!



Infrared Spectroscopy

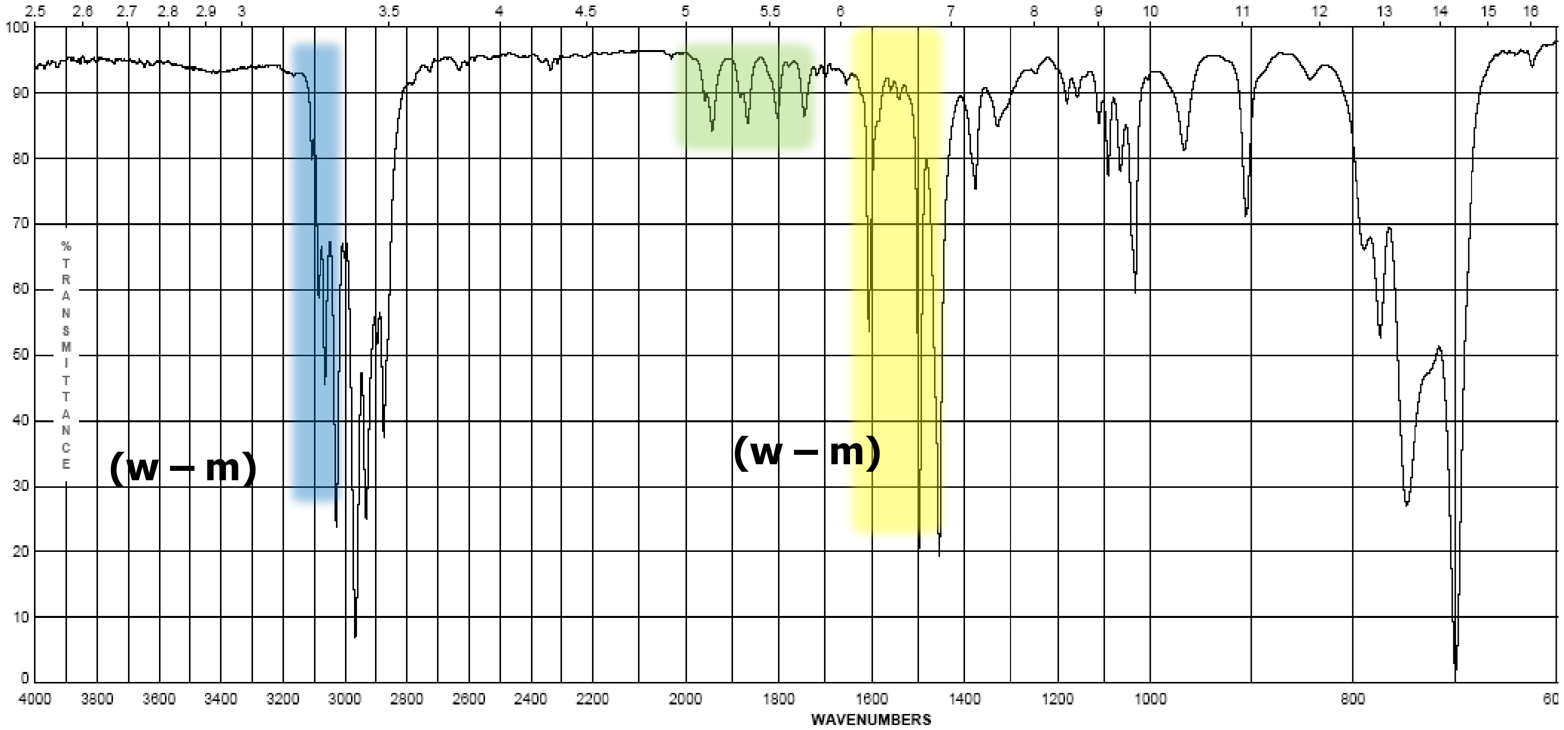
Ethyl benzene



4. Aromatics

- Due to the delocalization of e^- in the ring, C-C bond order is 1.5, the stretching frequency for these bonds is slightly lower in energy than normal C=C
- These show up as a ***pair*** of sharp bands, 1500 & 1600 cm^{-1}, (lower frequency band is stronger)

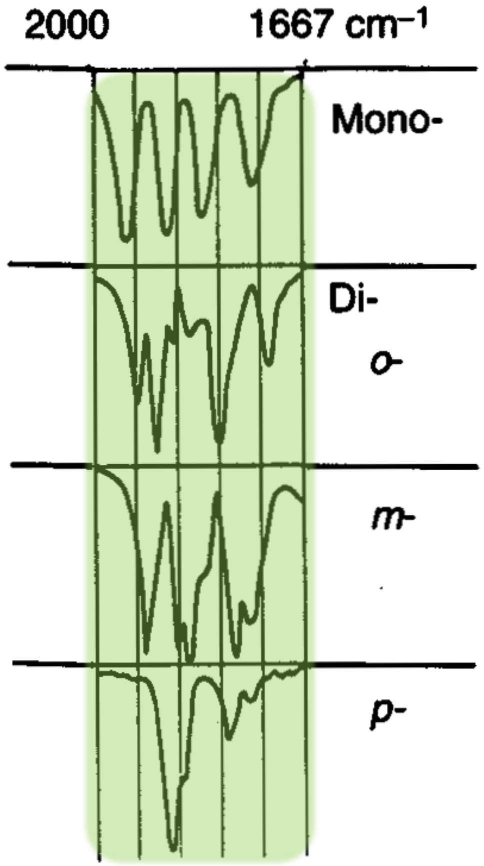
- C-H bonds off the ring show up similar to vinyl C-H at 3000-3100 cm^{-1}

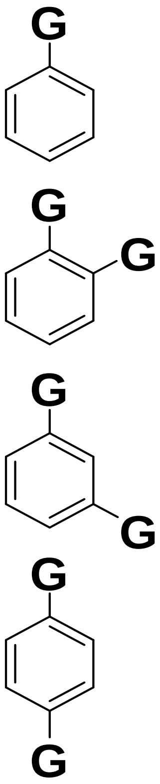


Infrared Spectroscopy

4. Aromatics

- If the region between 1667-2000 cm^{-1} (w) is free of interference (C=O stretching frequency is in this region) a weak grouping of peaks is observed for aromatic systems
- Analysis of this region, called the *overtone of bending* region, can lead to a determination of the substitution pattern on the aromatic ring





Monosubstituted

1,2 disubstituted (*ortho* or *o*-)

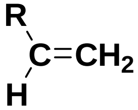
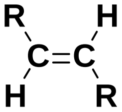
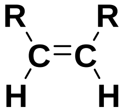
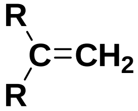
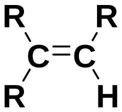
1,2 disubstituted (*meta* or *m*-)

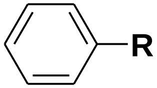
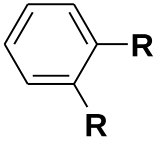
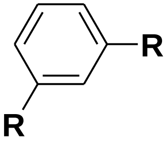
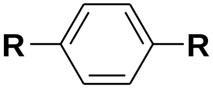
1,4 disubstituted (*para* or *p*-)

Infrared Spectroscopy

5. **Unsaturated Systems** – substitution patterns

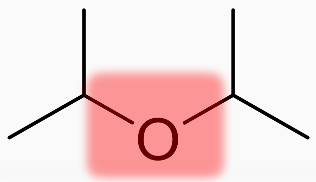
- The substitution of aromatics and alkenes can also be discerned through the out-of-plane bending vibration region
- However, other peaks often are apparent in this region. *These peaks should only be used for reinforcement of what is known or for hypothesizing as to the functional pattern.*

	cm^{-1}
	985-997 905-915
	960-980
	665-730
	885-895
	790-840

	cm^{-1}
	730-770 690-710
	735-770
	860-900 750-810 680-725
	800-860

Infrared Spectroscopy

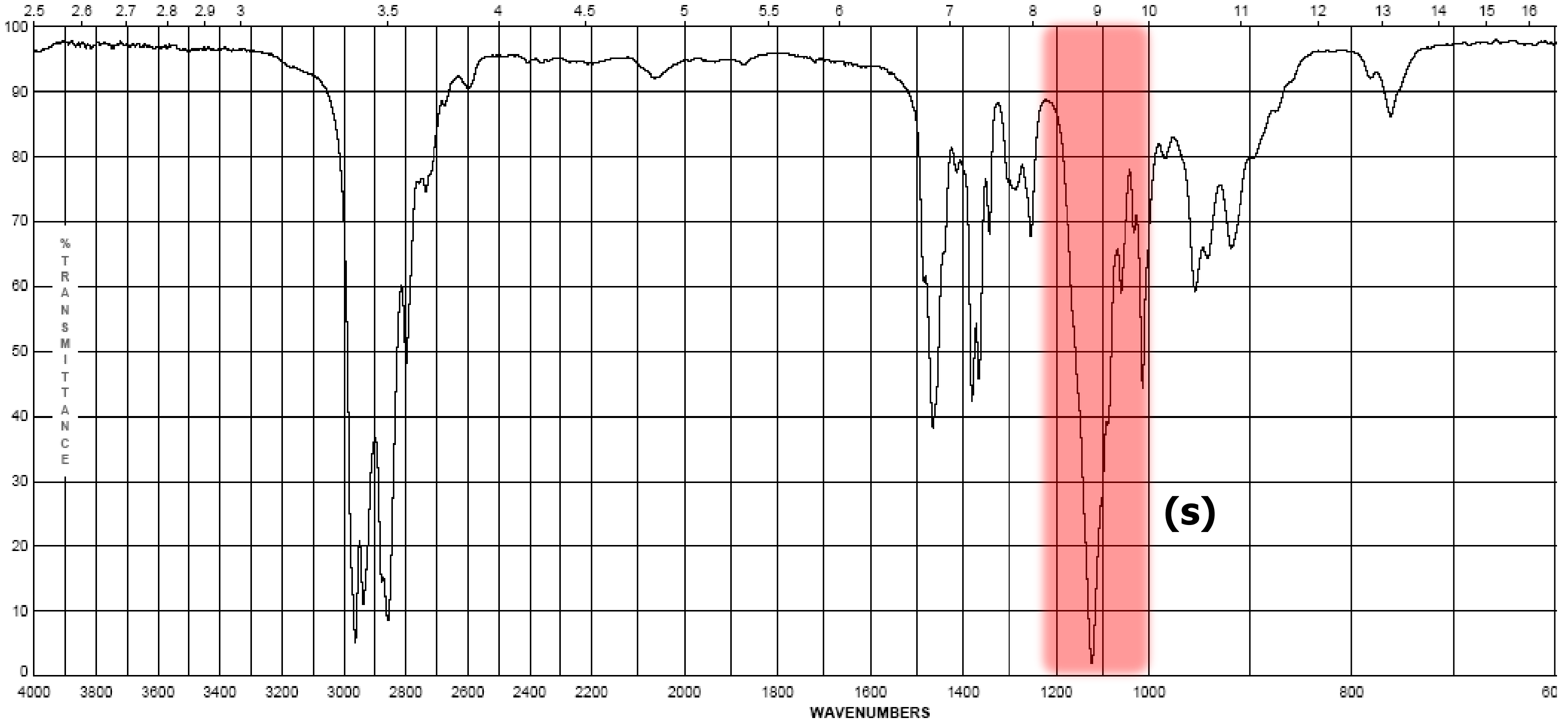
Diisopropyl ether



6. **Ethers** – addition of the C-O-C asymmetric band and vinyl C-H bonds

- Show a strong band for the antisymmetric C-O-C stretch at 1050-1150 cm^{-1}

- Otherwise, dominated by the hydrocarbon component of the rest of the molecule

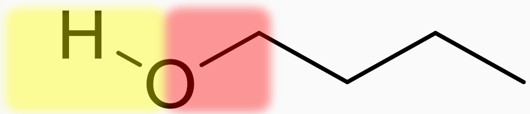


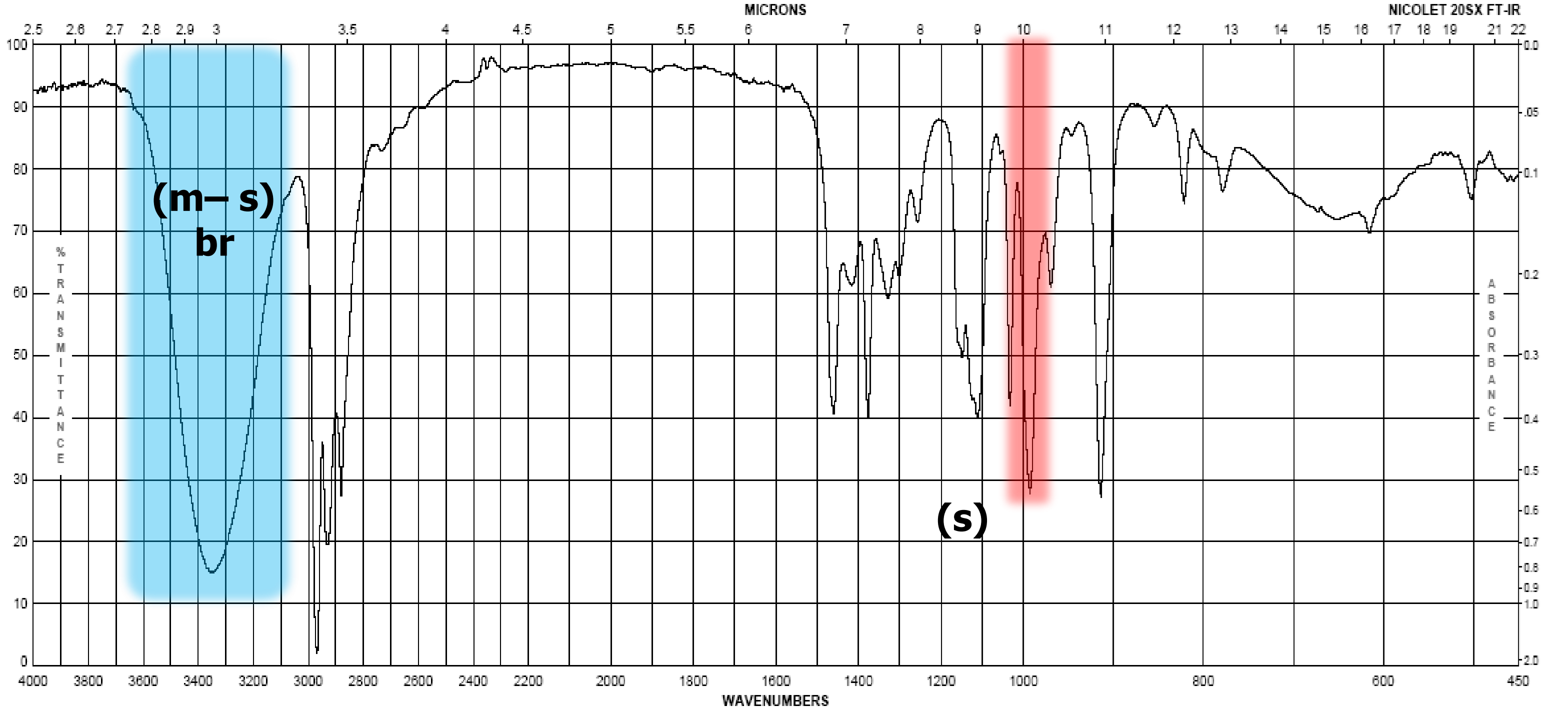
Infrared Spectroscopy

7. Alcohols

- Strong, broad O-H stretch from 3200-3400 cm^{-1}
- Like ethers, C-O stretch from 1050-1260 cm^{-1}
- Band position changes depending on the alcohols substitution: 1° 1075-1000; 2° 1075-1150; 3° 1100-1200; phenol 1180-1260
- The shape is due to the presence of hydrogen bonding

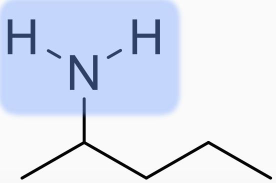
1-butanol





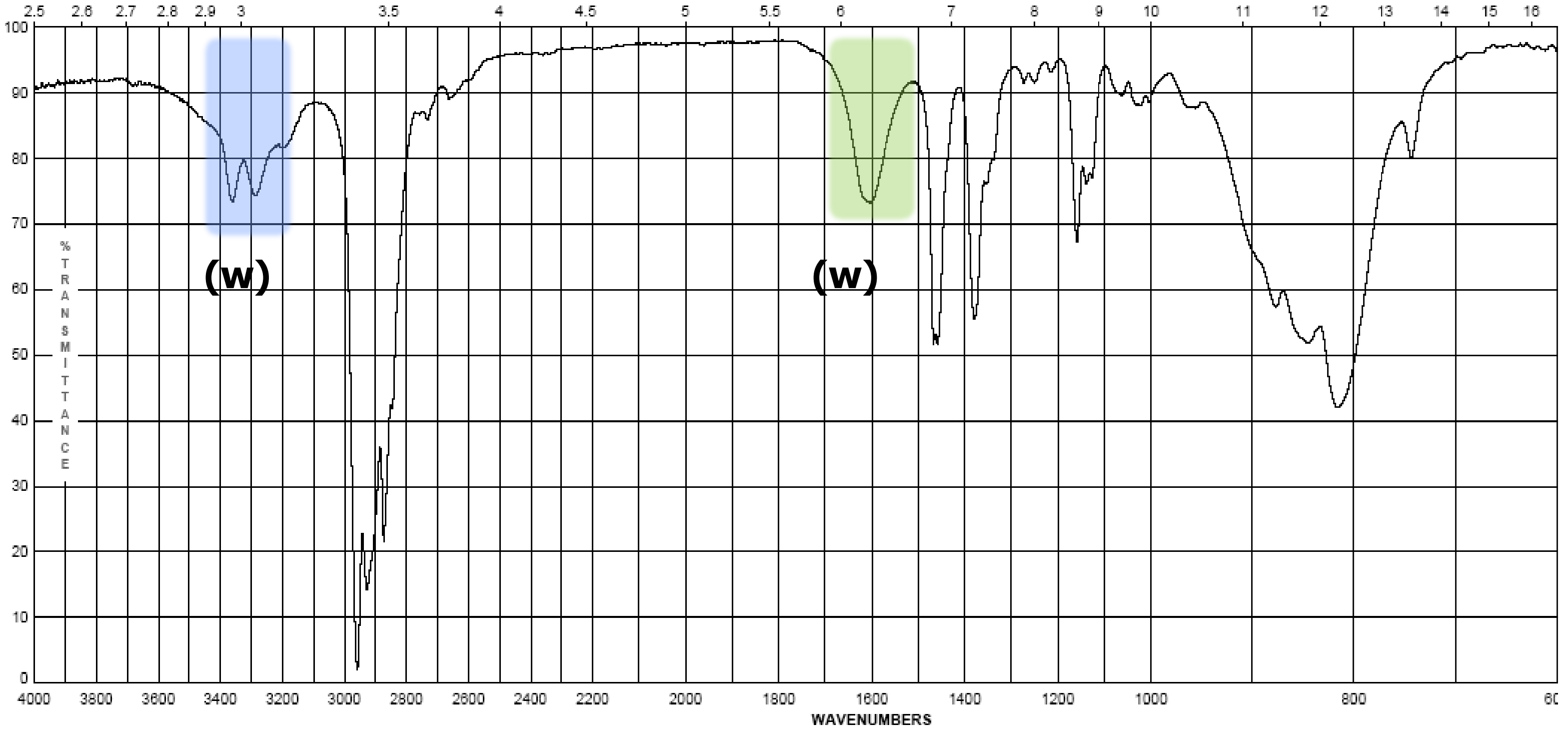
Infrared Spectroscopy

2-aminopentane



8. Amines - Primary

- Shows the –N-H stretch for NH_2 as a ***doublet*** between 3200-3500 cm^{-1} (symmetric and anti-symmetric modes)
- $-NH_2$ has deformation band from 1590-1650 cm^{-1}
- Additionally there is a “wag” band at 780-820 cm^{-1} that is not diagnostic



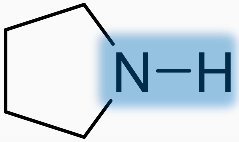
Infrared Spectroscopy

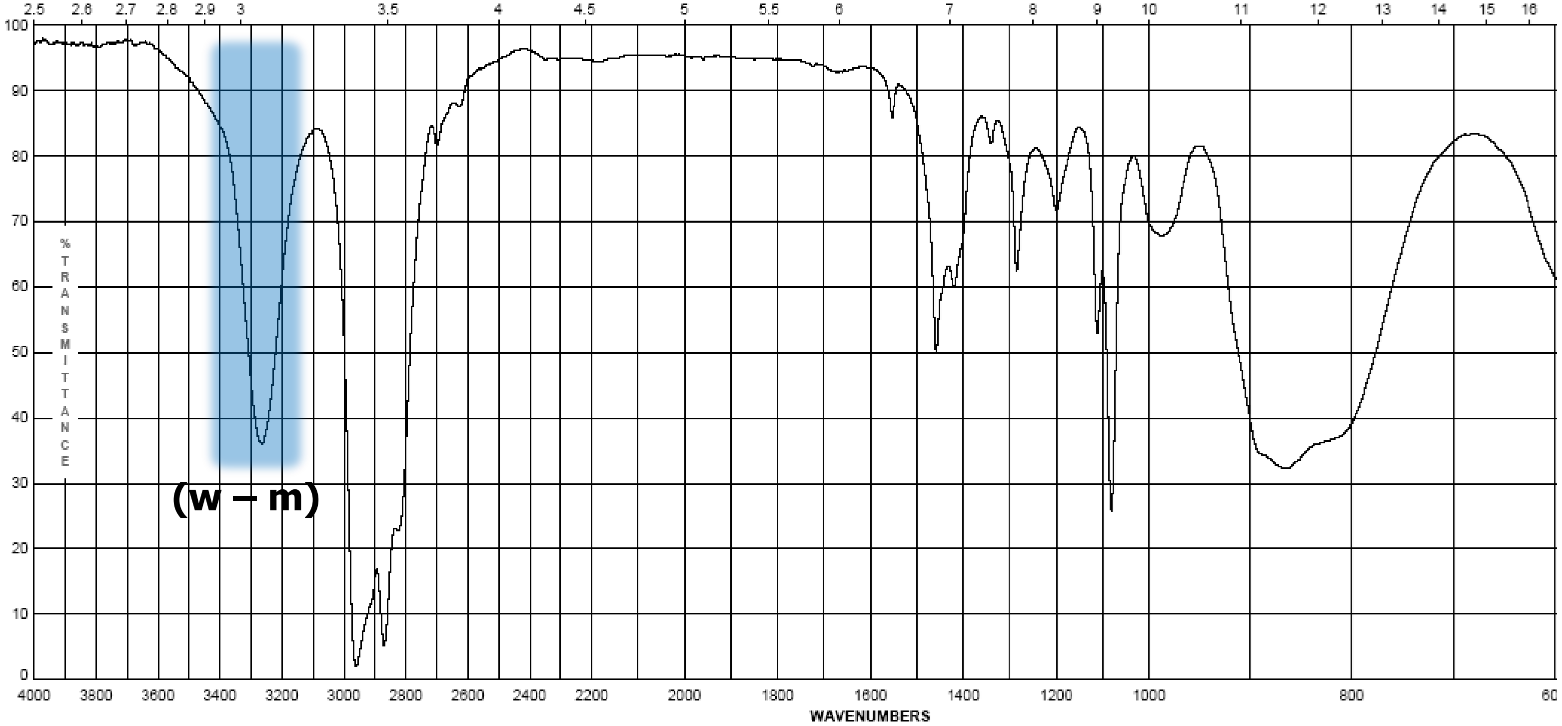
9. **Amines** – Secondary

- N-H band for R_2N-H occurs at 3200-3500 cm^{-1} as a single sharp peak weaker than –O-H

- Tertiary amines (R_3N) have no N-H bond and *will not* have a band in this region

pyrrolidine

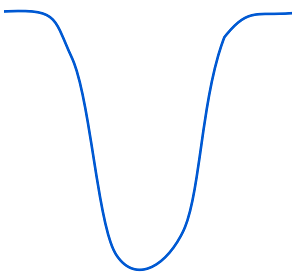




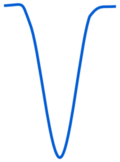
Infrared Spectroscopy

Pause and Review

- Inspect the bonds to H region (2700 – 4000 cm^{-1})
- Peaks from 2850-3000 are simply sp^3 C-H in most organic molecules
- Above 3000 cm^{-1} *Learn shapes, not wavenumbers!*:

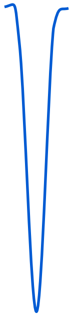


Broad U-shape peak
-**O—H** bond



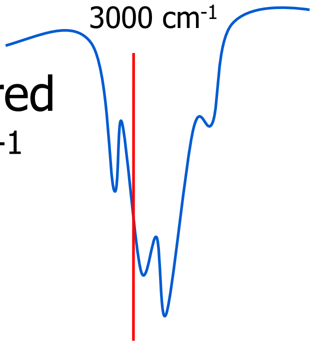
V-shape peak
-N—H bond for 2^o
amine (R$_2$**N—H**)

W-shape peak
-N—H bond for 1^o
amine (R**NH**$_2$)



Sharp spike
-C≡**C—H** bond

Small peak shouldered
just above 3000 cm^{-1}
C=**C—H** or Ph**—H**

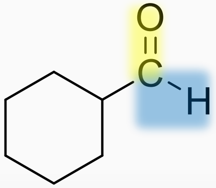


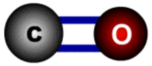
Infrared Spectroscopy

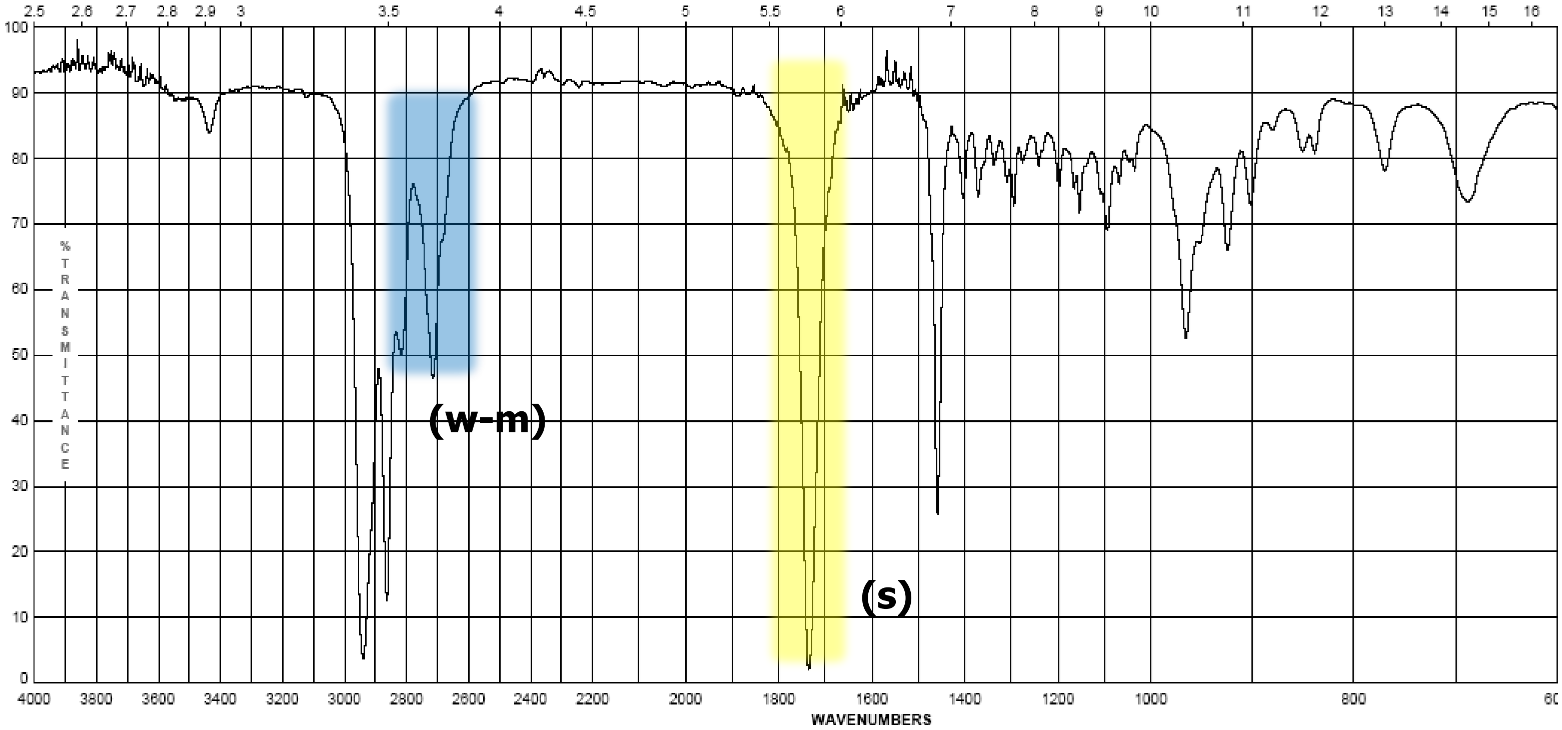
10. Aldehydes

- C=O (carbonyl) stretch from 1720-1740 cm^{-1}
- Band is sensitive to conjugation, as are all carbonyls (upcoming slide)
- A highly unique sp^2 C-H stretch appears as a doublet, 2720 & 2820 cm^{-1} called a "*Fermi doublet*"

Cyclohexyl carboxaldehyde

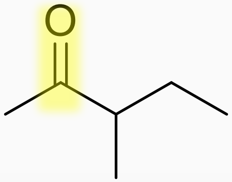






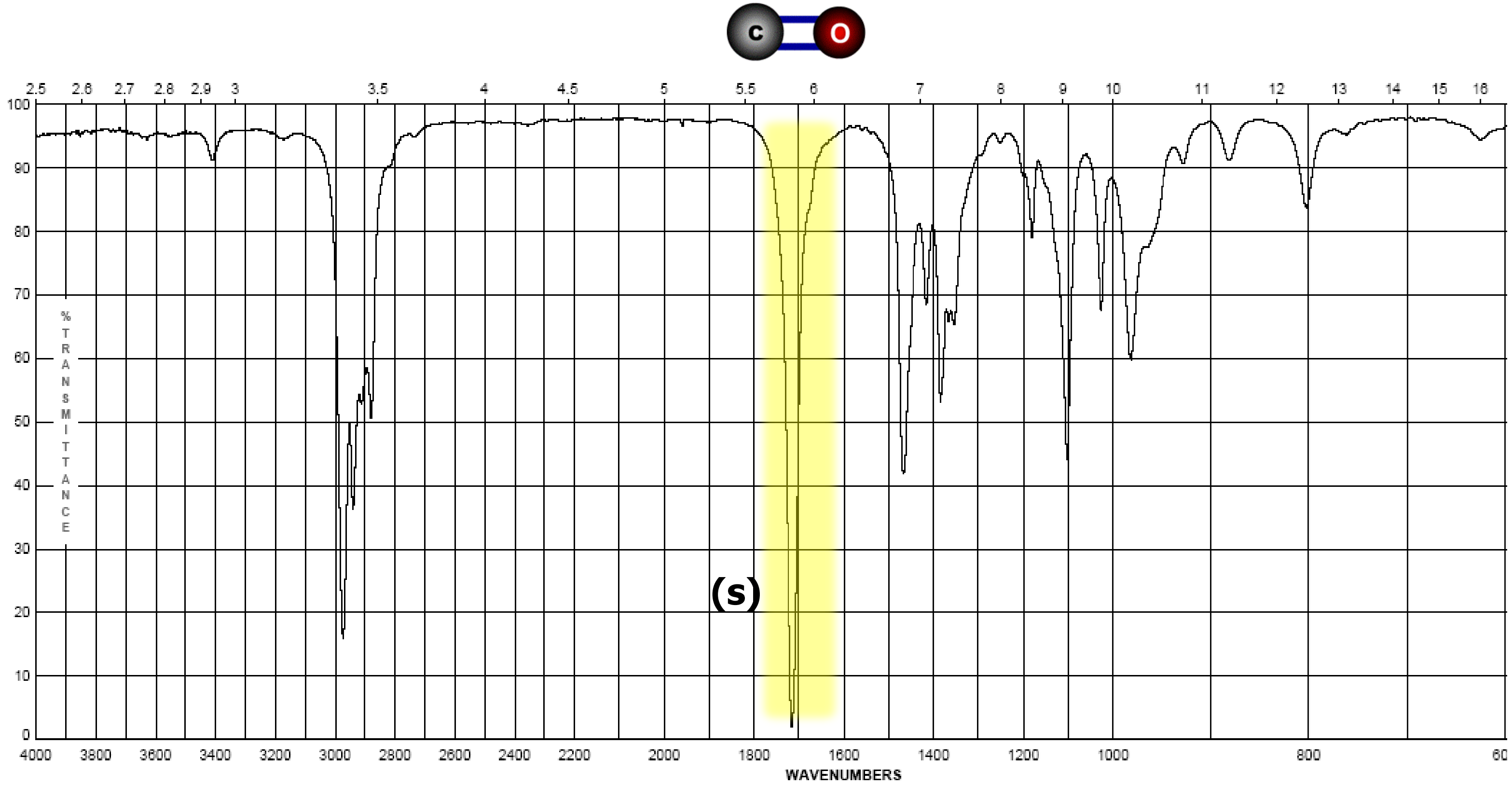
Infrared Spectroscopy

3-methyl-2-pentanone



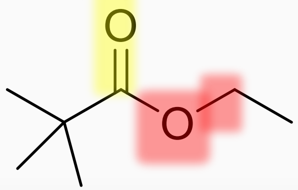
11. Ketones

- Simplest of the carbonyl compounds as far as IR spectrum – carbonyl only
- C=O stretch occurs at 1705-1725 cm^{-1}



Infrared Spectroscopy

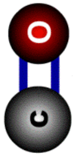
Ethyl pivalate

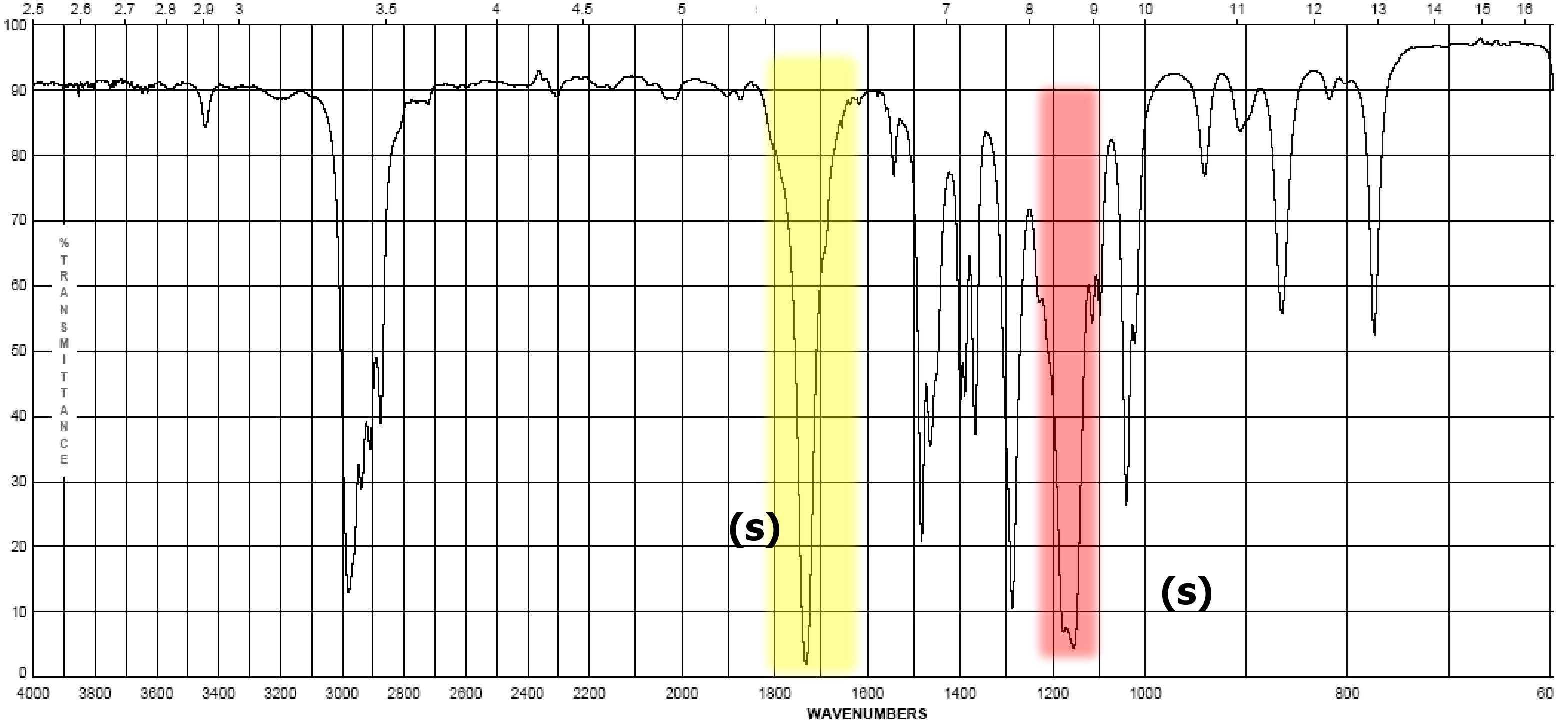


12. Esters

- C=O stretch at 1735-1750 cm^{-1}

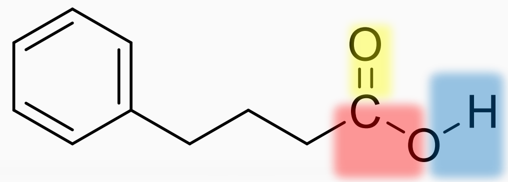
- Strong band for C-O at a higher frequency than ethers or alcohols at 1150-1250 cm^{-1}





Infrared Spectroscopy

4-phenylbutyric acid

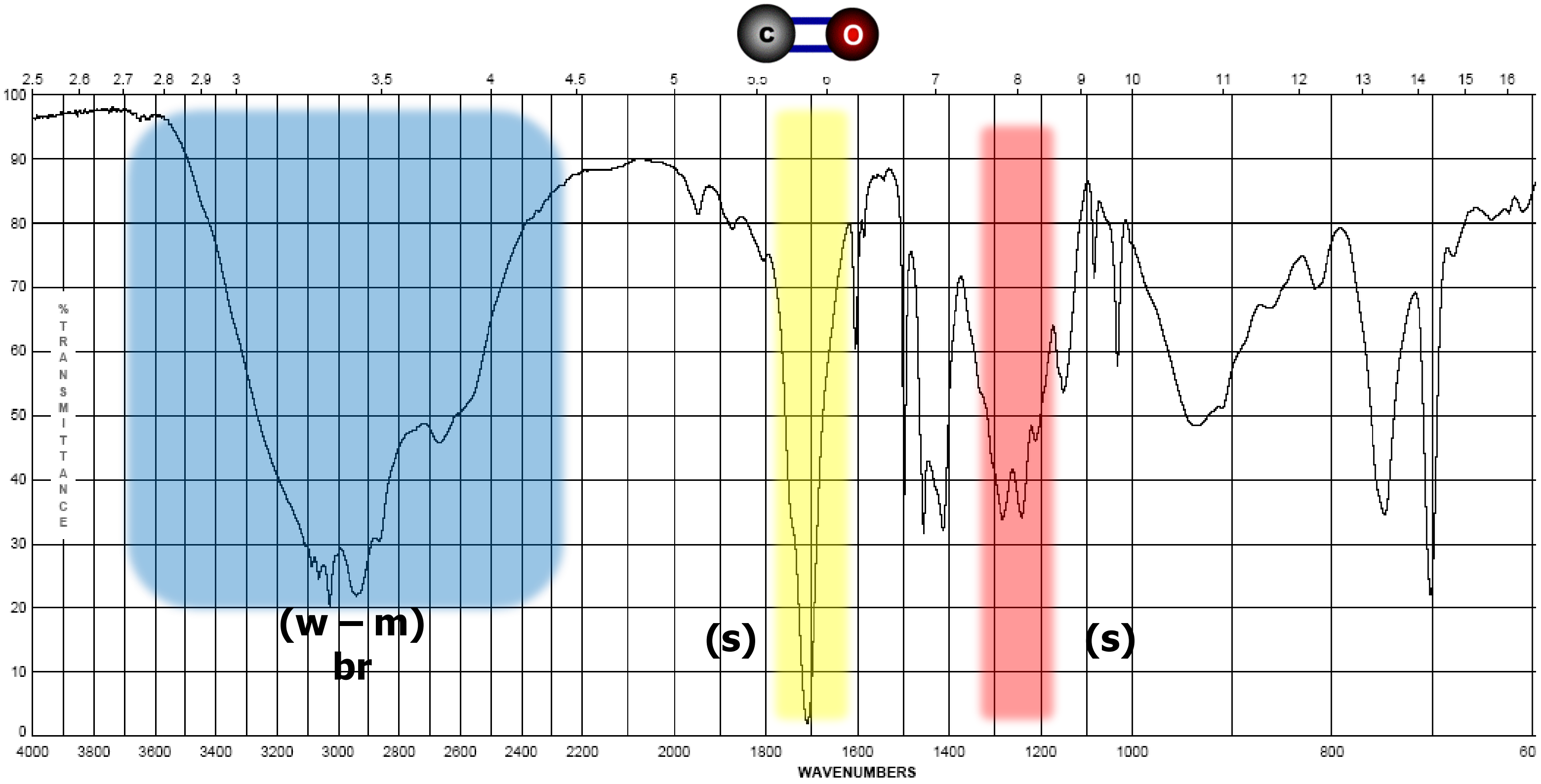


13. Carboxylic Acids:

- Gives the messiest of IR spectra

- C=O band occurs between 1700-1725 cm^{-1}

- The highly dissociated O-H bond has a broad band from 2400-3500 cm^{-1} covering up to half the IR spectrum in some cases



Infrared Spectroscopy

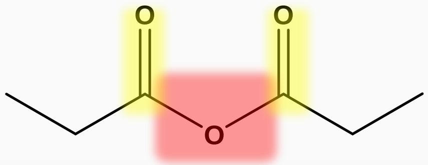
14. Acid anhydrides

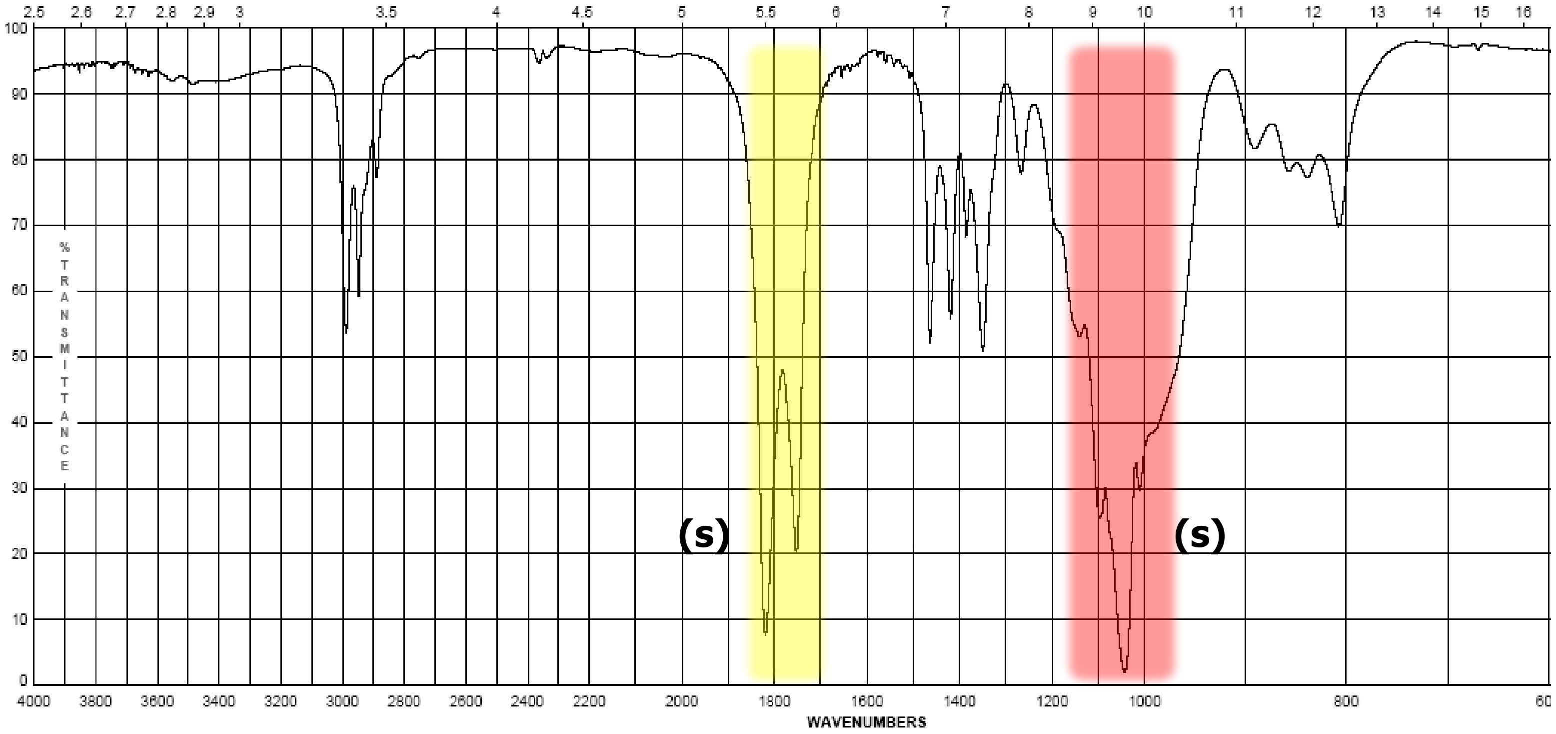
- Coupling of the anhydride though the ether oxygen splits the carbonyl band into two with a separation of 70 cm^{-1}

- Bands are at 1740-1770 cm-1 and 1810-1840 cm^{-1}

- Mixed mode C-O stretch at 1000-1100 cm^{-1}

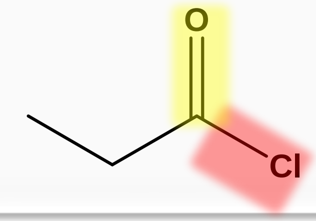
Propionic anhydride





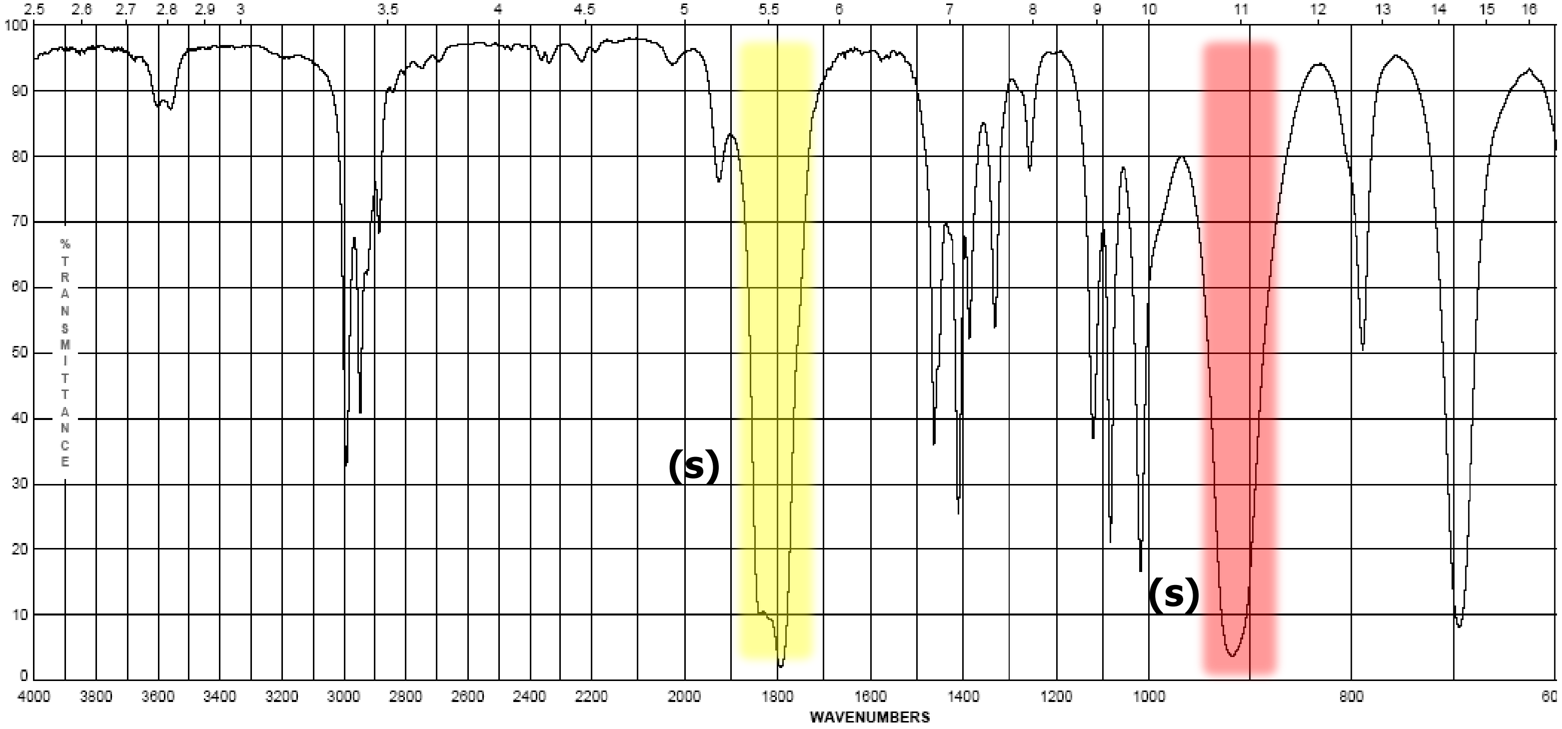
Infrared Spectroscopy

Propionyl chloride



15. Acid halides

- Clefted band at 1770-1820 cm^{-1} for C=O
- Bonds to halogens, due to their size (see Hooke's Law derivation) occur at low frequencies, only Cl is light enough to have a band on IR, C-Cl is at 600-800 cm^{-1}



Infrared Spectroscopy

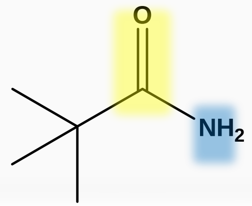
16. Amides

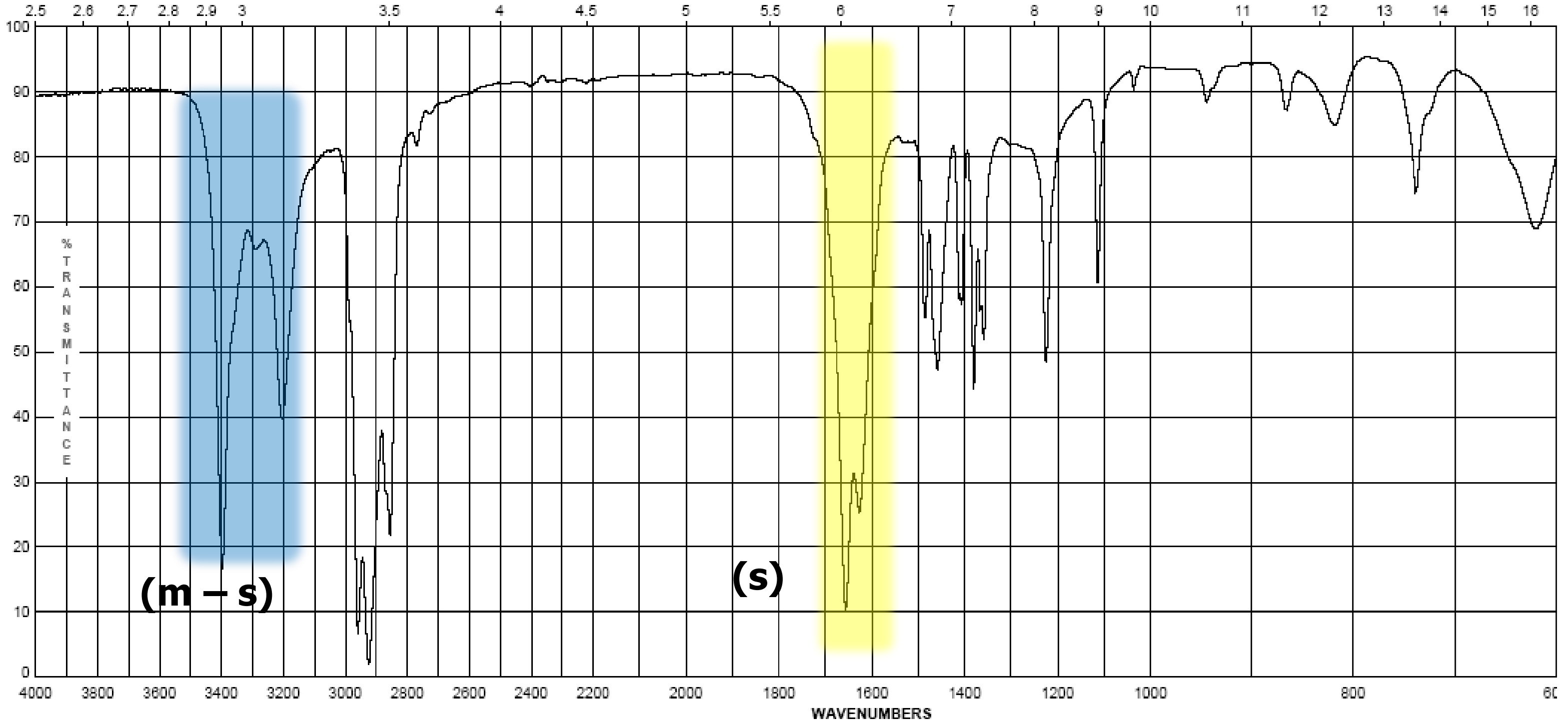
- Display features of amines and carbonyl compounds
- C=O stretch at 1640-1680 cm^{-1}

- If the amide is primary (-NH$_2$) the N-H stretch occurs from 3200-3500 cm^{-1} as a doublet

- If the amide is secondary (-NHR) the N-H stretch occurs at 3200-3500 cm^{-1} as a sharp singlet

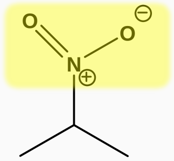
pivalamide





Infrared Spectroscopy

2-nitropropane

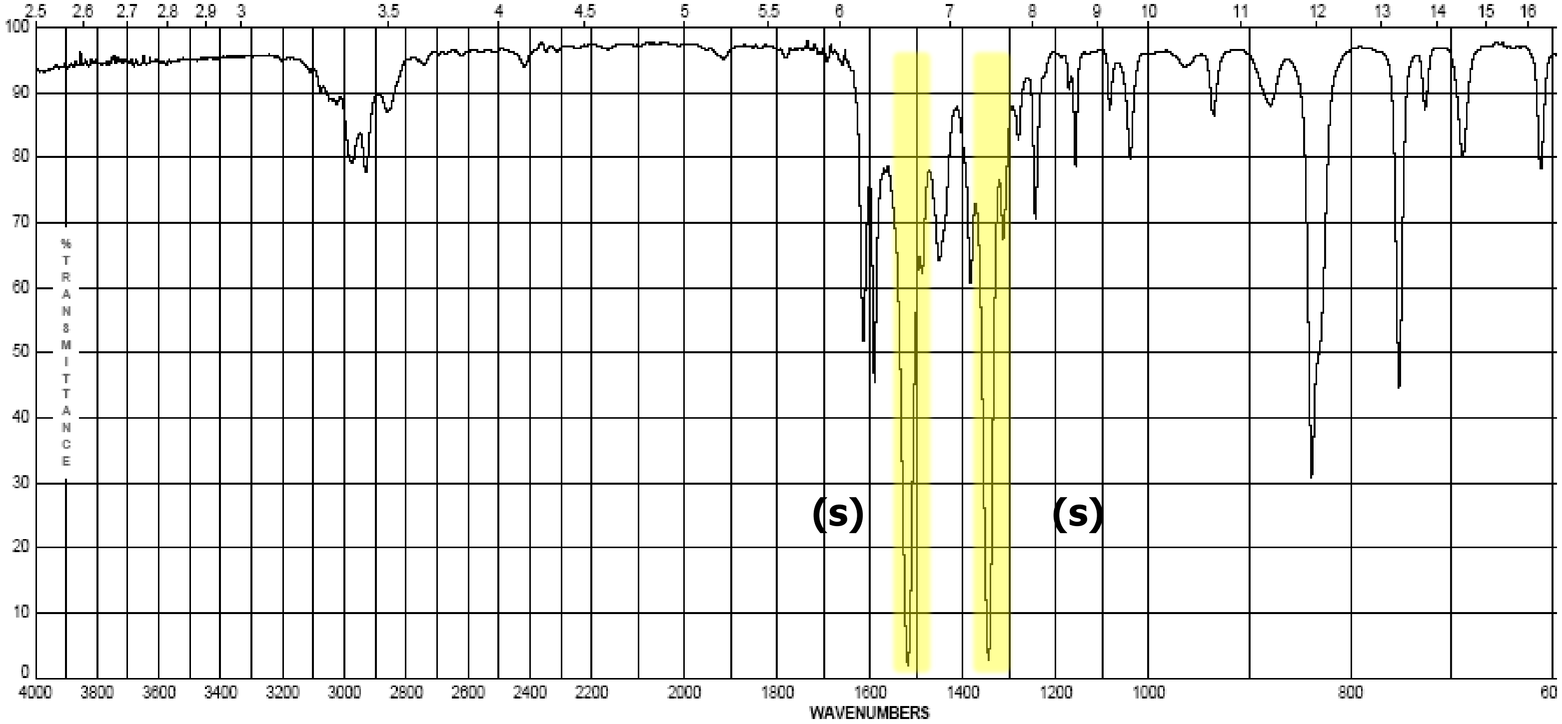


17. Nitro group (-NO_2)

- Proper Lewis structure gives a bond order of 1.5 from nitrogen to each oxygen

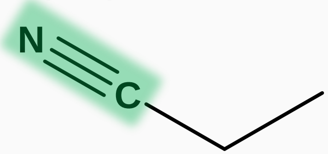
- Two bands are seen (symmetric and asymmetric) at 1300-1380 cm^{-1} and 1500-1570 cm^{-1}

- This group is a strong resonance withdrawing group and is itself vulnerable to resonance effects



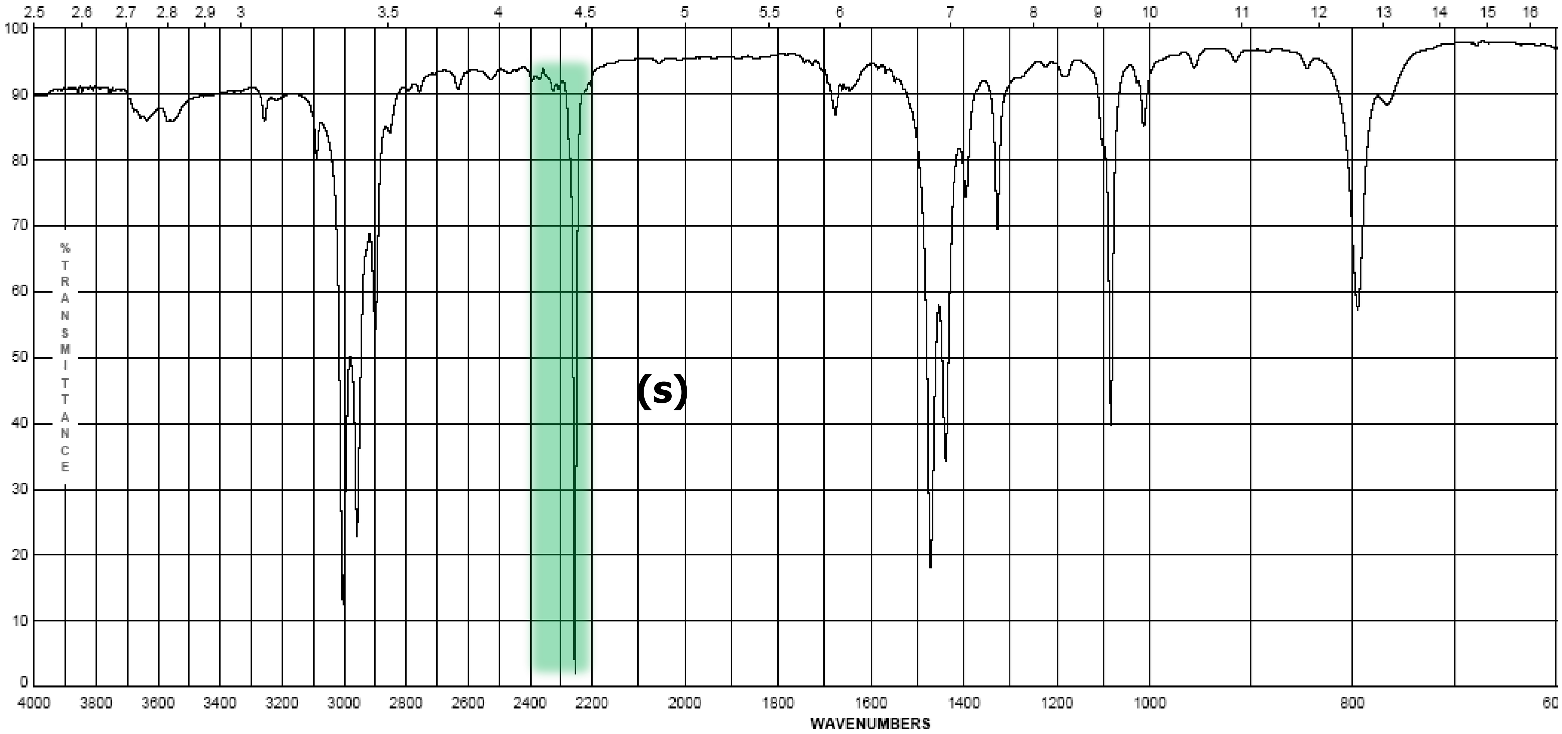
Infrared Spectroscopy

propionitrile



18. Nitriles (the cyano- or –C≡N group)

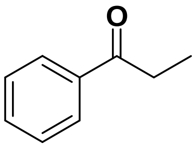
- Principle group is the carbon nitrogen triple bond at 2100-2280 cm^{-1}
- This peak is usually much more intense than that of the alkyne due to the electronegativity difference between carbon and nitrogen



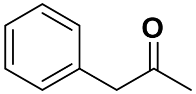
Infrared Spectroscopy

Effects on IR bands

1. **Conjugation** – by resonance, conjugation lowers the energy of a double or triple bond. The effect of this is readily observed in the IR spectrum:

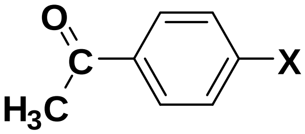


1684 cm^{-1}
C=O

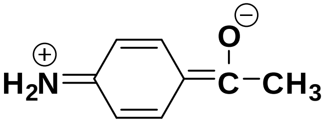


1715 cm^{-1}
C=O

- Conjugation will lower the observed IR band for a carbonyl from 20-40 cm^{-1} provided conjugation gives a strong resonance contributor

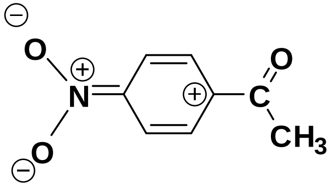


X =	NH_2	CH_3	Cl	NO_2	
	1677	1687	1692	1700	cm^{-1}



Strong resonance contributor

vs.



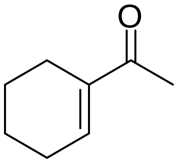
Poor resonance contributor
(cannot resonate with C=O)

- Inductive effects are usually small, unless coupled with a resonance contributor (note –CH_3 and –Cl above)

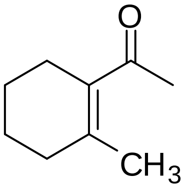
Infrared Spectroscopy

Effects on IR bands

2. **Steric effects** – usually not important in IR spectroscopy, unless they reduce the strength of a bond (usually π) by interfering with proper orbital overlap:



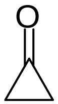
C=O: 1686 cm^{-1}



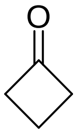
C=O: 1693 cm^{-1}

   - Here the methyl group in the structure at the right causes the carbonyl group to be slightly out of plane, interfering with resonance

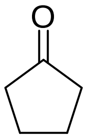
3. **Strain effects** – changes in bond angle forced by the constraints of a ring will cause a slight change in hybridization, and therefore, bond strength



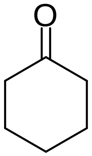
1815 cm^{-1}



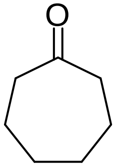
1775 cm^{-1}



1750 cm^{-1}



1715 cm^{-1}



1705 cm^{-1}

   - As bond angle decreases, carbon becomes more electronegative, as well as less sp^2 hybridized (bond angle < 120°)

Infrared Spectroscopy

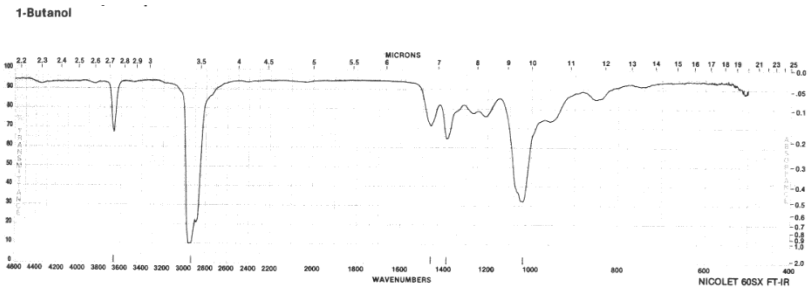
Infrared Spectroscopy

Effects on IR bands

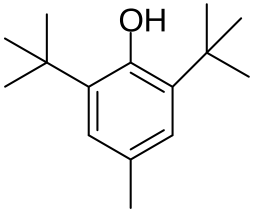
4. Hydrogen bonding

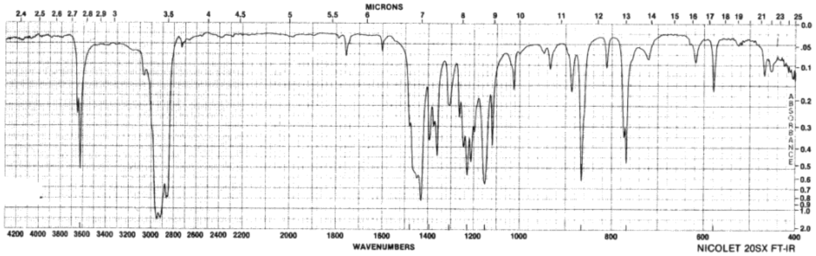
- Hydrogen bonding causes a broadening in the band due to the creation of a continuum of bond energies associated with it
- In the solution phase these effects are readily apparent; in the gas phase where these effects disappear or in lieu of steric effects, the band appears as sharp as all other IR bands:

Gas phase spectrum of 1-butanol

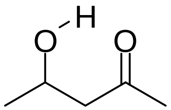


Steric hindrance to H-bonding in a di-*tert*-butylphenol





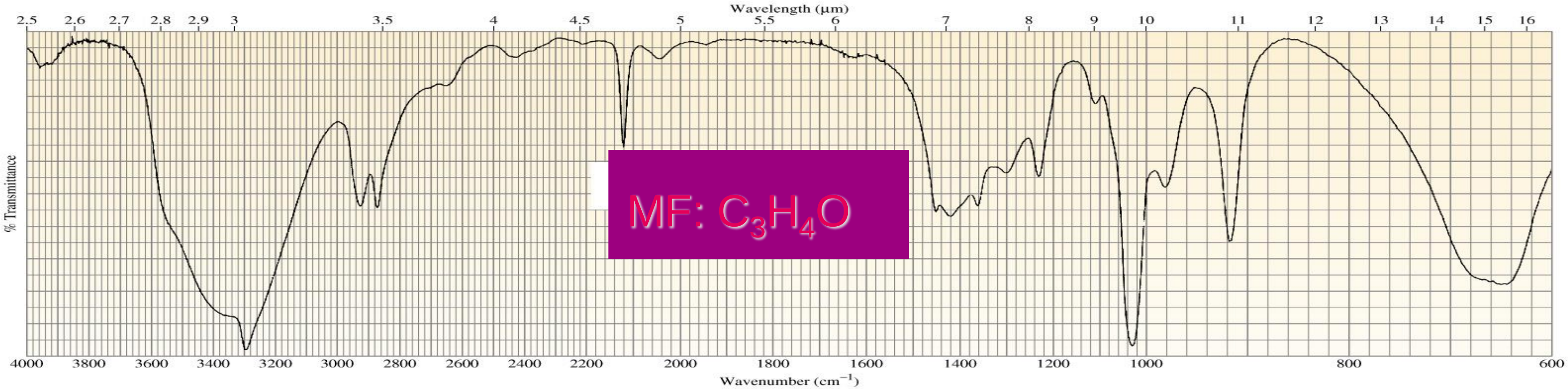
- H-bonding can interact with other functional groups to lower frequencies



C=O; 1701 cm^{-1}

Question ?

Question ?



MF: C_3H_4O

Identify the compound from the IR above.

A) Cyclopropanone
B) propynol
C) acrylaldehyde
D) propenoic acid

References Books:

1. Orgnanic Spectroscopy by P.S. Kalsi (4th Edition),
2. Spectroscopy by Jagamohan ((3rd Edition)
3. Organic Spectroscopy by Pavia (4th Edition)
4. Molecular Spectroscopy by D. Satyanarana
5. Instrumental Methods of Chemical Analysis by B.K. Sharma

Solid State and Structural Chemistry.

Ms. Y. S. Munavalli
PG, Dept of Chemistry

Classification of Solids:

In a solid substance, the constituent particles are held together by strong forces of attraction, and because of this, the particles of solids are packed in proper order or symmetry. Therefore, a solid has a definite shape, a distinct boundary, a fixed volume, and negligible compressibility. Some solids are strong, while some solids may break under force. In this article, we will explore different classifications of solids.

Solids have been classified as crystalline solids and amorphous solids. Let's study about both these types in detail.

CRYSTALLINE SOLIDS

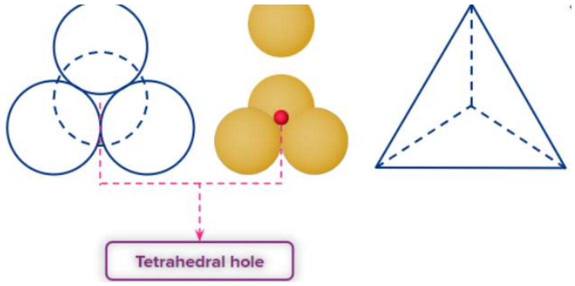
The solids having sharp edges and well-defined planes are called crystals or crystalline solids. Crystalline solids are also called true solids. Sodium chloride, quartz, gold, copper, and iron are some examples of crystalline solids.

AMORPHOUS SOLID STATE

Amorphous solid-state comprises those solids which have the property of rigidity and incompressibility but to a certain extent. They do not have a definite geometrical form or long range of order. Examples include glass, rubber, plastic, etc.

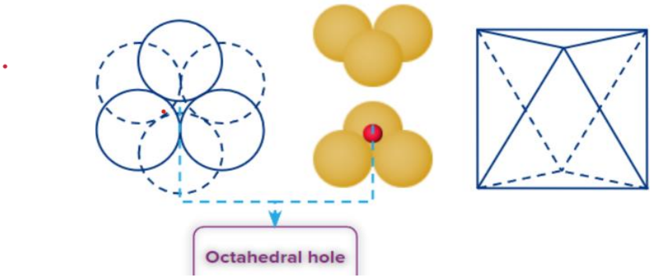
TETRAHEDRAL VOID

The void formed by 4 constituent particles (atoms, molecules and ions) is called tetrahedral void. Take 4 atoms and arrange three of them in one plane and one above the plane. The vacant space between these atoms will be in the shape of a tetrahedron. The coordination number of tetrahedral void is 4 as void is surrounded by 4 neighbouring atoms.

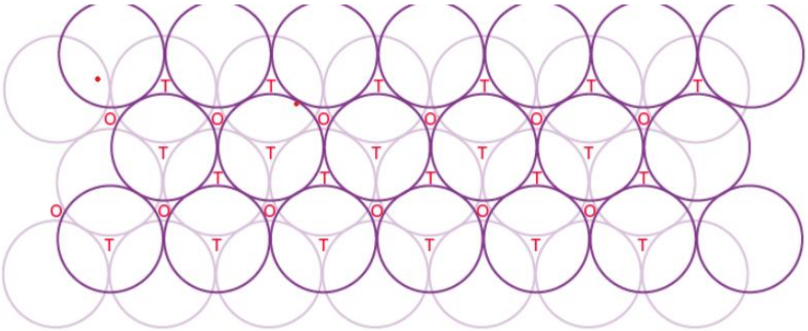


Octahedral Void

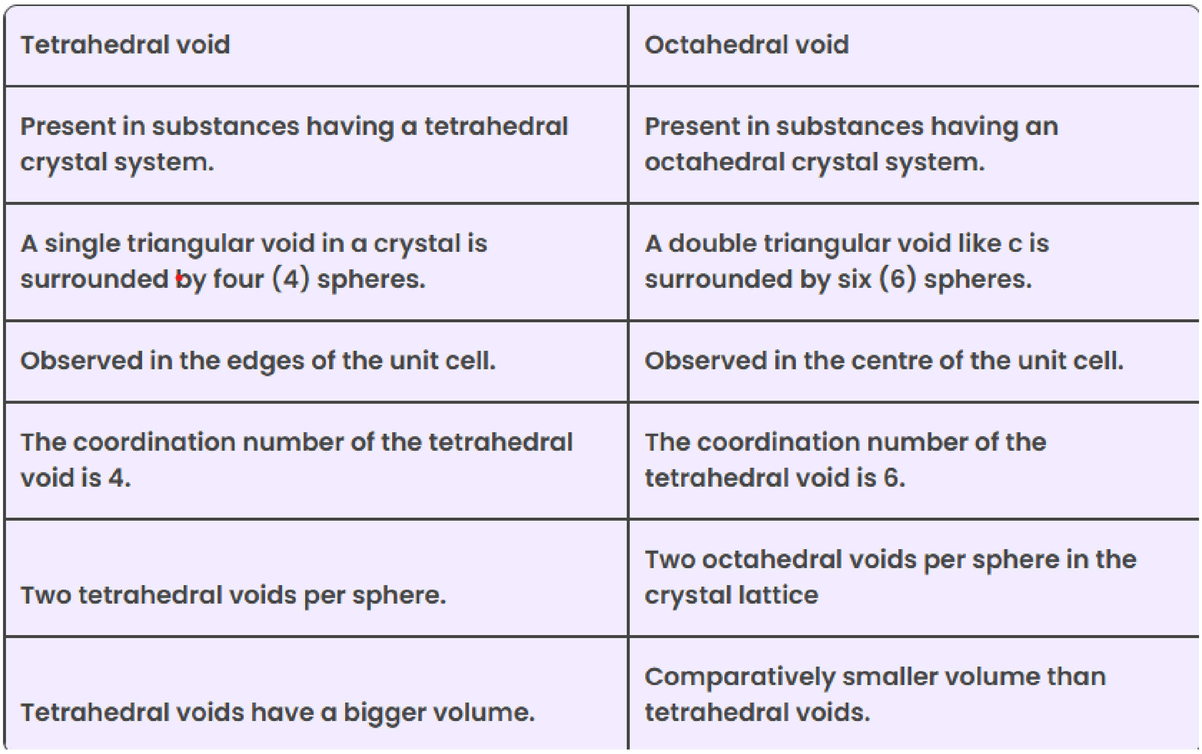
The void formed by 6 constituent particles (atoms, molecules and ions) is called an octahedral void. Take 3 atoms in one plane and arrange them in a triangular shape, then put another 3 atoms on top of the previous arrangement in opposite direction. The vacant space between them will be in the shape of an octahedron. The coordination number is 6 as void is surrounded by 6 neighbouring atoms.



Tetrahedral and octahedral voids



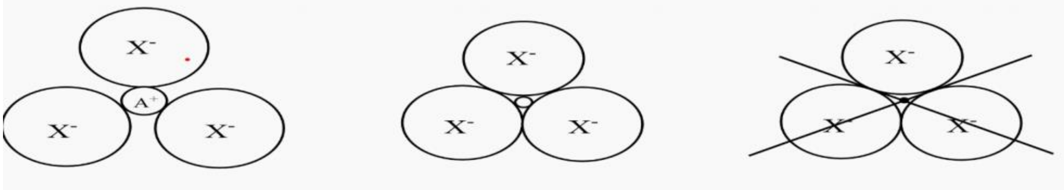
Differences between Tetrahedral and Octahedral Void



Tetrahedral void	Octahedral void
Present in substances having a tetrahedral crystal system.	Present in substances having an octahedral crystal system.
A single triangular void in a crystal is surrounded by four (4) spheres.	A double triangular void like c is surrounded by six (6) spheres.
Observed in the edges of the unit cell.	Observed in the centre of the unit cell.
The coordination number of the tetrahedral void is 4.	The coordination number of the tetrahedral void is 6.
Two tetrahedral voids per sphere.	Two octahedral voids per sphere in the crystal lattice
Tetrahedral voids have a bigger volume.	Comparatively smaller volume than tetrahedral voids.

Radius ratio rule

When the coordination number is 3 in an ionic compound AX, 3 X^- ions are in contact with one A^+ ion. A limiting case arises when the X^- are in contact with one another. By simple geometry, this gives the ratio (radius A^+/radius X^-) = 0.155. This is the lower limit for a coordination number of three. If the radius ratio is less than 0.155, then the positive ion is not in contact with the negative ions, and it rattles in the holes, and the structure is unstable. As the differences in the sizes of the ions increase,the radius ratio alsoincreases.



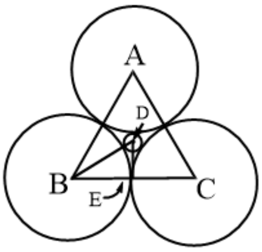
Sizes of ions for coordination number 3

.

Calculation Of Some Limiting Radius Ratio Values

Coordination number 3 (planar triangle)

The smaller positive ions with radius r+ interacted with 3 larger negative ions with radius r-. Plainly $AB=BC=AC=2r^{-}$, $BE=r^{-}$, $BD=r^{+} + r^{-}$, the angle D-B-E is 30^{o}.



$\cos 30^{\circ} = BE/BD$

$BD = BE/\cos 30^{\circ}$

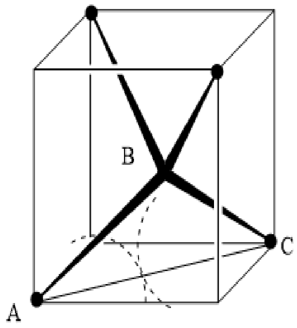
$r^{+} + r^{-} = r^{-} /\cos 30^{\circ} = r^{-}/0.866 = r^{-} \times 1.155$

$r^{+} = (1.155r^{-}) – r^{-} = 0.155r^{-}$

$r^{+}/r^{-} = 0.155$

Coordination number 4 (tetrahedral)

Tetrahedral arrangement inscribed in a cube. The angle ABC is the tetrahedral angle of $109^{o}28'$ and hence the angle ABD is half of this, that is $54^{o}.44'$. In the triangle ABD:



$\text{Sin ABD} = 0.8164 = \frac{AD}{AB} = \frac{r^{-}}{r^{+} + r^{-}}$

Taking reciprocals

$\frac{r^{+}+r^{-}}{r^{-}} + \frac{1}{0.8164} + 1.225$

Rearranging

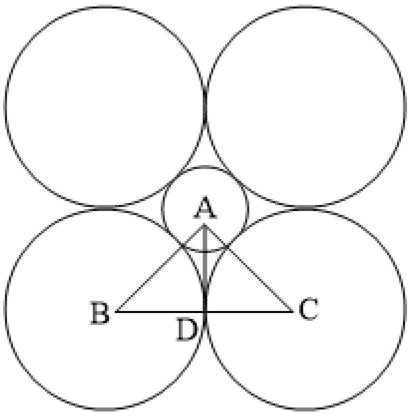
$r^{+} / r^{-} + 1 = 1.225$

Hence,

$r^{+} / r^{-} = 0.225$

Coordination number 6 (octahedral)

The smaller positive ion of radius r+ touches six larger negative ions of radius r-. In the triangle ABD



$$\text{Cos ABD} = 0.7071 = \frac{BD}{AB} = \frac{r^-}{r^+ + r^-}$$

Taking reciprocals

$$\frac{r^+ + r^-}{r^-} + \frac{1}{0.7071} + 1.414$$

Rearranging

$$r^+ / r^- + 1 = 1.414$$

Hence,

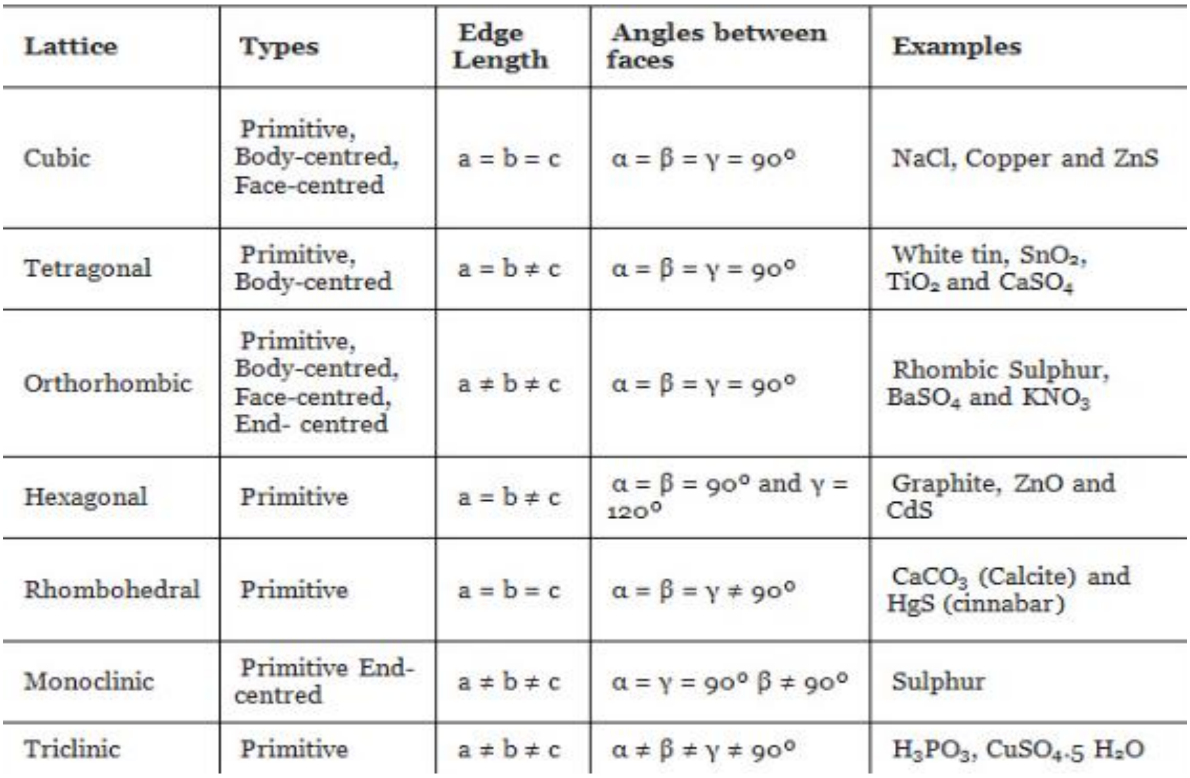
$$r^+ / r^- = 0.414$$

The corresponding limiting radius ratio values for coordination numbers 2, 3, 4, 6, and 8 are:

Limiting Radius Ratio	Coordination number of cation	Shape	Examples
<0.155	2	Linear	
0.155-0.225	3	Planer triangle	Boron oxide
0.225-0.414	4	Tetrahedral	ZnS
0.414-0.732	6	Octahedral	NaCl
0.732-0.999	8	Body-centered cubic	CsCl

Bravais Lattices.

Bravais Lattice refers to the ***14 different 3-dimensional configurations into which atoms can be arranged in crystals.*** The smallest group of symmetrically aligned atoms which can be repeated in an array to make up the entire crystal is called a **unit cell**.



Lattice	Types	Edge Length	Angles between faces	Examples
Cubic	Primitive, Body-centred, Face-centred	$a = b = c$	$\alpha = \beta = \gamma = 90°$	NaCl, Copper and ZnS
Tetragonal	Primitive, Body-centred	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$	White tin, SnO_2, TiO_2 and $CaSO_4$
Orthorhombic	Primitive, Body-centred, Face-centred, End- centred	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90°$	Rhombic Sulphur, $BaSO_4$ and KNO_3
Hexagonal	Primitive	$a = b \neq c$	$\alpha = \beta = 90°$ and $\gamma = 120°$	Graphite, ZnO and CdS
Rhombohedral	Primitive	$a = b = c$	$\alpha = \beta = \gamma \neq 90°$	$CaCO_3$ (Calcite) and HgS (cinnabar)
Monoclinic	Primitive End-centred	$a \neq b \neq c$	$\alpha = \gamma = 90°$ $\beta \neq 90°$	Sulphur
Triclinic	Primitive	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90°$	H_3PO_3, $CuSO_4.5\ H_2O$

SPINELS

Spinel is a name of Mixed Ore of Magnesium(Mg) and Aluminium(Al), its molecular formula is $MgAlO_4$ ($MgO.Al_2O_3$). Here Mg is in +2 oxid. state and Al is in +3 oxid. state.

So, in general we can say Spinels are AB_2X_4 type complexes.

where, A= any dipositive metal (eg. Mg^{+2}, Ni^{+2})

B= any tripositive metal (eg. Fe^{+3}, Al^{+3}, La^{+3})

X = O, S, Se, etc.

- No. of Tetrahedral (Td) voids per unit cell = 8
- No. of Octahedral (Oh) voids per unit cell = 4

TYPES OF SPINELS:

On the basis of position occupied by $\mathbf{A^{+2}}$ ions and $\mathbf{B^{+3}}$ ions, spinels are of two types:

Normal Spinel:

The divalent **A^{+2}** ions occupy the tetrahedral voids, whereas the trivalent **B^{+3}** ions occupy the octahedral voids in the close packed arrangement of oxide ions. A normal spinel can be represented as: **$(A^{+2})^{tet}(B^{+3})_2^{oct}O_4$**
e.g. Mn_3O_4,$ZnFe_2O_4$,$FeCr_2O_4$

Inverse Spinel:

The **A^{+2}** ions occupy the octahedral voids, whereas half of **B^{+3}** ions occupy the tetrahedral voids.
It can be represented as: $(B^{+3})^{tet}(A^{+2}B^{+3})^{oct}O_4$ E.g. Fe_3O_4 (ferrite), $CoFe_2O_4$, $NiFe_2O_4$ etc.

Prediction Of Structure OfSpinels:

basic rule for determining whether a complex is Normal or Inverse Spinel

- **For Normal Spinel:**

CFSE of **B^{+3}** ions in Octahedral Field> CFSE of **B^{+3}** ions in Tetrahedral Field

>CFSE of **A^{+2}** ions in Octahedral Field
>CFSE of **A^{+2}** ions in Tetrahedral Field

[i.e. if CFSE of B^{+3} ions in Octahedral fieldis largest of all CFSE]

For Inverse Spinel:

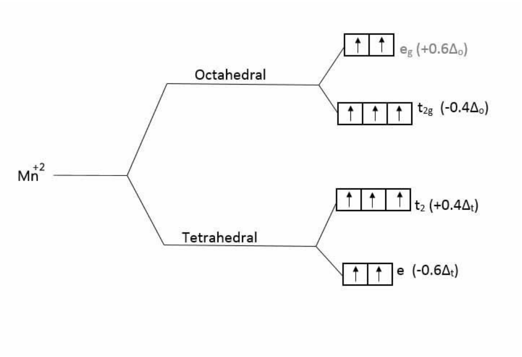
CFSE of **A^{+2}** ions in Octahedral felid> CFSE of **A^{+2}** ions in Tetrahedral field

>CFSE of **B^{+3}** ions in Octahedral felid
>CFSE of **B^{+3}** ions in Tetrahedral field

[i.e. if CFSE of A^{+2} ions in Octahedral fieldis largest of all CFSE]

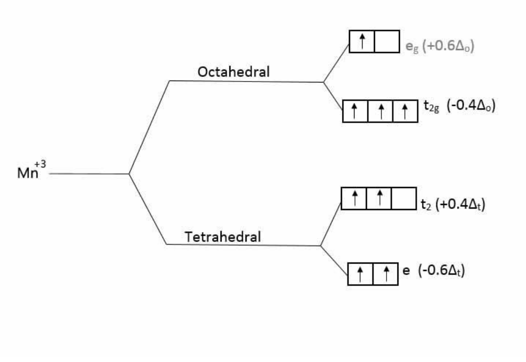
Let's take an example of Mn_3O_4

Here Mn_3O_4 exist as $Mn.Mn_2O_4$, therefore Mn exists in +2 and +3 oxidation state.



CFSE of Mn^{+2} in octahedral field = $0\Delta_o$

CFSE of Mn^{+2} in tetrahedralfield = $0\Delta_t$



CFSE of Mn^{+3} in octahedral field = $-0.6\Delta_0$

CFSE of Mn^{+3} in tetrahedral field = $-0.4\Delta_t$

here CFSE of Mn^{+3} in Oh field is more than all, therefore is Mn_3O_4 Normal Spinel

Rules:

1. If both **A^{+2}** and **B^{+3}** are non-transition metals then spinel will be NORMAL.
2. If **A^{+2}** is Non transition metal and **B^{+3}** is transition metal (having d^1 d^2 d^3 d^4 d^6 d^7 d^8 d^9) then spinel will be NORMAL.
3. If is transition metal with (d^1 d^2 d^3 d^4 d^6 d^7 d^8 d^9) and B is also transition metal with (d^0 d^5 and d^{10}) system then spinel will be INVERSE.

Exception:

- **$NiAl_2O_4$** for which the formula can be written as $(Al_{0.75}Ni_{0.25})^{tet}$ $[Ni_{0.75}Al_{1.25}]^{octa}O_4$ is a Random Defected Inverse Spinel. The CFSE of Ni^{II} is greater in octahedral than tetrahedral coordination. But Al^{3+} also has strong preference for octahedral sites due to high lattice energy. This leads to almost complete randomization of all the cations on all the available sites. Its formula can be written as $(Al_{0.75}Ni_{0.25})^{tet}$ $[Ni_{0.75}Al_{1.25}]^{octa}O_4$.

EXAMPLES FOR SPINEL AND INVERSE SPINEL STRUCTURES

1) $MgAl_2O_4$ is a normal spinel since both the divalent and trivalent ions are non transition metal ions. There is no question of CFSE.

2) **Mn_3O_4 is a normal spinel** since the Mn^{2+} ion is a high spin d^5 system with zero LFSE. Whereas, Mn^{3+} ion is a high spin d^4 system with considerable LFSE.

3) **Fe_3O_4 is an inverse spinel** since the Fe(III) ion is a high spin d^5 system with zero CFSE. Whereas the divalent Fe(II) is a high spin d^6 system withmore CFSE.

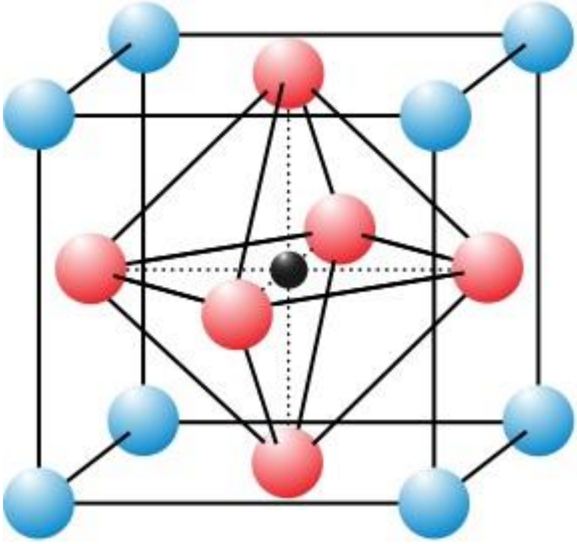
4) **$NiFe_2O_4$ is again an inverse spinel** since the divalent Ni^{2+} (a d^8 ion) has more CFSE than the trivalent Fe^{3+} (a d^5 ion).

5) **$FeCr_2O_4$ is a normal spinel** since the divalent Fe^{2+} is a high spin d^6 ion with CFSE = 4 Dq and the trivalent Cr^{3+} is a high spin d^3 ion with CFSE = 12 Dq. Hence Cr^{3+} gets more CFSE while occupying octahedral sites.

6) **Co_3O_4 is a normal spinel**. Even in the presence of weak field oxo ligands, the Co^{3+} is a low spin d^6 ion with very high CFSE. It is due to high charge on Co^{3+}. Hence all the Co^{3+} ions occupy the octahedral sites.

PEROVSKITE STRUCTURE

A **perovskite** is any material of formula ABX_3 with a crystal structure similar to that of the mineral perovskite, which consists of calcium titanium oxide ($CaTiO_3$) 'A' and 'B' are two positively charged ions (i.e. cations), often of very different sizes, and X is a negatively charged ion (an anion, frequently oxide) that bonds to both cations. The 'A' atoms are generally larger than the 'B' atoms. The ideal cubic structure has the B cation in 6-fold coordination, surrounded by an octahedron of anions, and the A cation in 12-fold cuboctahedral coordination. Additional perovskite forms may exist where both/either the A and B sites have a configuration of $A1_{x-1}A2_x$ and/or $B1_{y-1}B2_y$ and the X may deviate from the ideal coordination configuration as ions within the A and B sites undergo changes in their oxidation states.



Four general categories of cation-pairing are possible: $A^{+}B^{2+}X^{-}_3$, or 1:2 perovskites;[8] $A^{2+}B^{4+}X^{2-}_3$, or 2:4 perovskites; $A^{3+}B^{3+}X^{2-}_3$, or 3:3 perovskites; and $A^{+}B^{5+}X^{2-}_3$, or 1:5 perovskites.

DEFECTS OF SOLIDS

Point defects explain about the **imperfections of solids** along with the types of point defects. Crystalline solids are formed by joining many small crystals. Different types of defects are found in crystals after the process of crystallization.

Point defects are accounted for when the crystallization process occurs at a very fast rate. These defects mainly happen due to deviation in the arrangement of constituting particles. In a crystalline solid, when the ideal arrangement of solids is distorted around a point/ atom it is called a point defect.

There are 3 types of point defects:

1. **Stoichiometric defect**
2. **Frenkel defect**
3. **Schottky defect**

1. Stoichiometric Defect:

In this kind of point defect, the ratio of positive and negative ions (Stoichiometric) and electrical neutrality of a solid is not disturbed. Sometimes it is also known as intrinsic or thermodynamic defects.

Fundamentally, they are of two types:

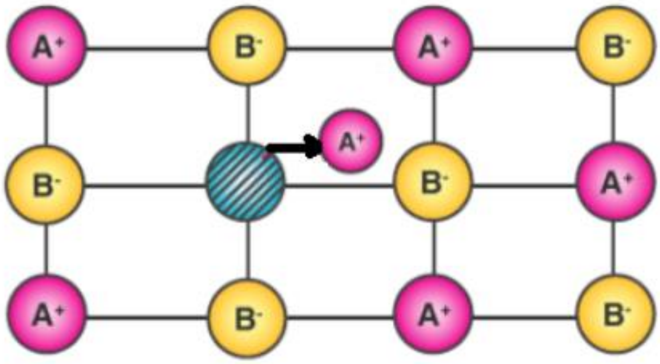
- ***Vacancy defect:*** When an atom is not present at their lattice sites, then that lattice site is vacant and it creates a vacancy defect. Due to this, the density of a substance decreases.
- ***Interstitial defect:*** It is a defect in which an atom or molecule occupies the intermolecular spaces in crystals. In this defect, the density of the substance increases.

A non-ionic compound mainly shows vacancy and interstitial defects. An ionic compound shows the same in Frenkel and Schottky defect.

2. Frenkel Defect:

In ionic solids generally, the smaller ion (cation) moves out of its place and occupies an intermolecular space. In this case, a vacancy defect is created on its original position and the interstitial defect is experienced at its new position.

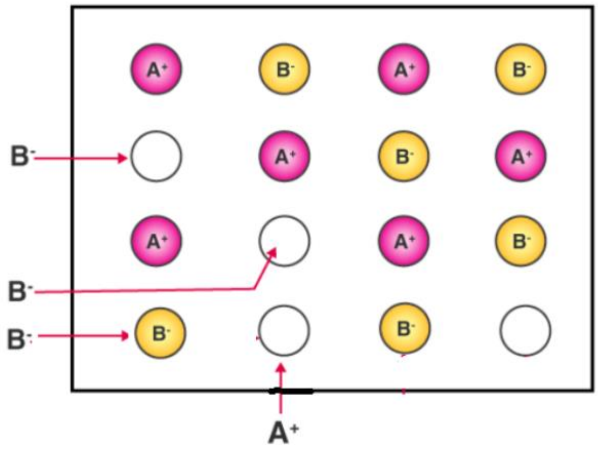
- It is also known as dislocation defect.
- The density of a substance remains unchanged.
- It happens when there is a huge difference in the size of anions and cations.
- ***Example:*** ZnS and AgCl.



Frenkel Defect

3. Schottky Defect

- This kind of vacancy defects is found in Ionic Solids. But in ionic compounds, we need to balance the electrical neutrality of the compound so an equal number of anions and cations will be missing from the compound.
- It reduces the density of the substance.
- In this, the size of cations and anions are of almost the same.



1. **<u>Impurity Defect:</u>** Let's understand the impurity defect by an example. If molten NaCl is crystallized with $SrCl_2$ compound then the Sr^{2+} ions replace two Na^+ ions and occupy the place of one Na^+ In this way the lattice site of one Na^+ is vacant and it creates an impurity defect.

2. **Non-Stoichiometric Defect:** In this defect, the cations and anions ratio is disturbed either because of adding or removing of ions.

<u>Types of Non-Stoichiometric Defect:</u>

1. ***Metal deficiency defect:*** In this, the solids have less number of metals relative to the described Stoichiometric proportion.

2. ***Metal excess defect:*** There are two types of metal excess defect:

- *<u>Metal excess defect due to anionic vacancies</u>:* This occurs due to the absence of anions from its original lattice site in crystals. Therefore, instead of anions, electrons occupy their position

- *<u>Metal excess defect due to the presence of extra cations at interstitial sites</u>:* Here, on heating the compound, it releases extra cations. These cations occupy the interstitial sites in crystals and the same number of electrons goes to neighbouring interstitial sites.

Reference:

1. Solid State Chemistry by D. K. Chakrabarti (2nd Edition).
2. West, Anthony R. (2004). *Solid State Chemistry and Its Applications*. John Wiley and Sons. ISBN 981-253-003-7.

Flame Photometry

Dr. M B Patil

3-The subsequent loss of energy will result in the movement of excited atoms to the low energy ground state with emission of some radiations as a wavelengths. The emitted wavelengths are specific for specific elements.

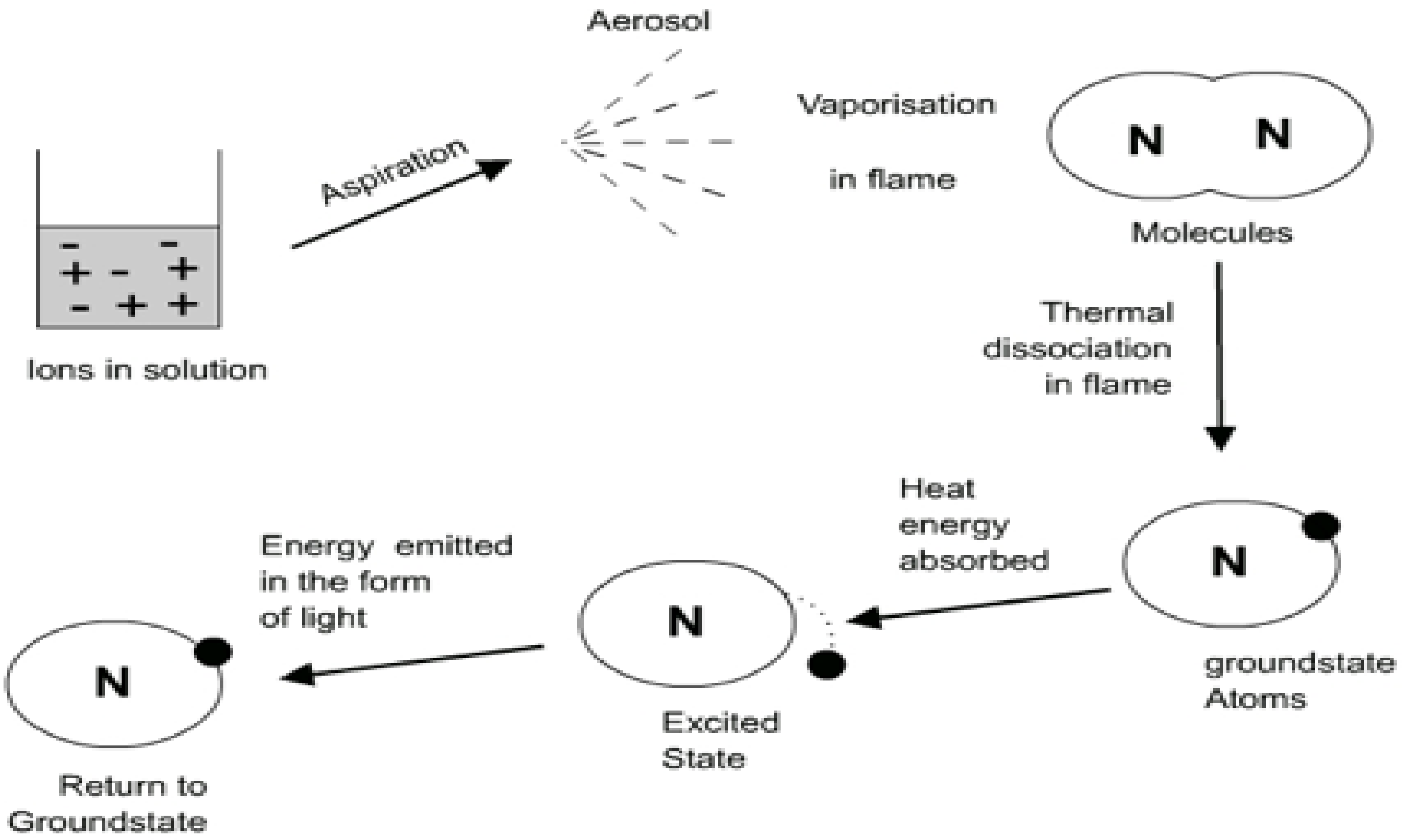


Fig 2: Brief overview of the process

1. The solution containing metal to be measure is first aspirated into the burner.

2. The solvent then evaporated leaving fine divided solid particles.

3. This solid particles move towards the flame, where the gaseous atoms and ions are produced.

4. The ions absorb the energy from the flame and excited to high energy levels.

5. When the atoms return to the ground state radiation of the characteristic element is emitted.

6. The intensity of emitted light is related to the concentration of the element.

Name of the element	**Emitted wavelenght range (nm)**	**Observed colour of the flame**
Potassium (K)	766	Violet 
Lithium (Li)	670	Red 
Calcium (Ca)	622	Orange 
Sodium (Na)	589	Yellow 
Barium (Ba)	554	Lime green 

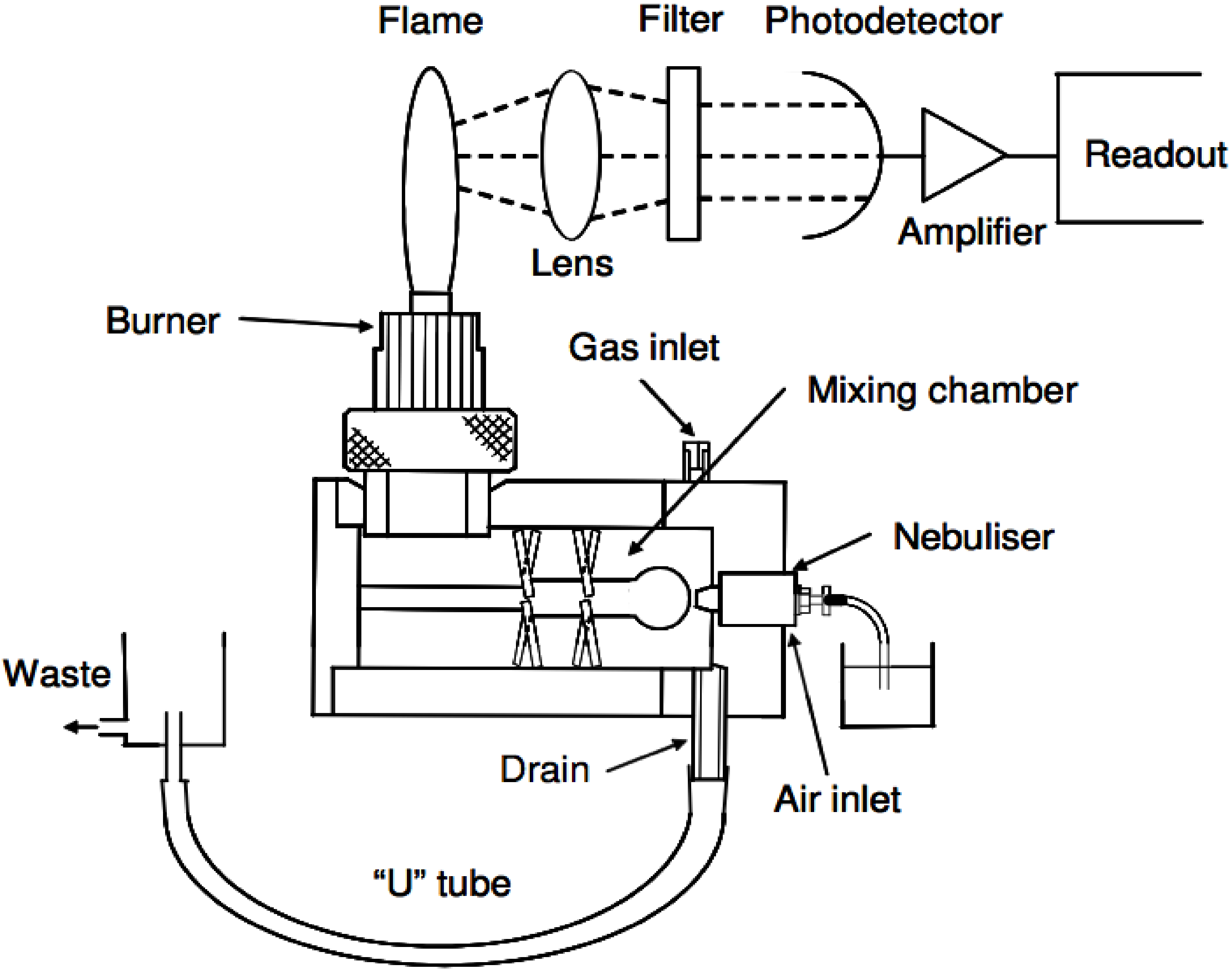
FP Components

1- Flame : A burner that provides flame and can be maintained in a constant form and at a constant temperature.

2- Nebuliser and mixing chamber: Helps to transport the homogeneous solution of the substance into the flame at a steady rate.

3- Monochromator : helps in isolating the wavelength to be measured from that of any other extraneous emissions.

4. Photo detector: Detect the emitted light and measure the intensity of radiation emitted by the flame. That is, the emitted radiation is converted to an electrical signal with the help of photo detector. The produced electrical signals are directly proportional to the intensity of light.


Flame
Filter
Photodetector
Readout
Lens
Amplifier
Burner
Gas inlet
Mixing chamber
Nebuliser
Waste
Drain
Air inlet
"U" tube

Flame (burner)

- Burner used in FP should have the following properties:

- The flame should have ability to evaporate the solvent to give a residue(deposit)

- It should convert this residue to gases state atom and finally into individual atoms

❖ The effect of flame depend on the temperature of flame and this temperature can be monitored by following method:

- Fuel to air ratio
- Type of solvent for preparing sample solution
- Amount of solvent which is entering to flame
- Type of burner used in FP

Flame (burner)

- Flame photometry employs a variety of fuels mainly air, oxygen or nitrous oxide (N_2O) as oxidant.
- Burners are of two types:

Total Consumption Burner and Premix or Laminar flow Burner.

The various processes in the flame are discussed below:

- **Desolvation**: The liquid solvent is evaporated, and the metal particles are dehydrated by the flame
- **Vapourisation:** The sample vaporises to a gas .

- **Atomization:** Reduction of metal ions in the solvent to metal atoms by the flame heat.

- **Excitation:** The electrostatic force of attraction between the electrons and nucleus of the atom helps them to absorb a particular amount of energy. The atoms then jump to the exited energy state.

- **Emission process:** Since the higher energy state is unstable the atoms jump back to the stable low energy state with the emission of energy in the form of radiation of characteristic wavelength, which is measured by the photo detector.

Types of FP

1- Direct type:

Standard solution of Na & K are atomised or aspirated into flame to provide a series of meter readings in which our unknown is going to compared with.

Direct type disadvantages

- 1- Any minor fluctuations in air, gas pressure might change response of instrument and then cause errors.
- 2- Separate analyses and sometimes separate solutions must be made for Na and K.

2- Internal standard method:

Another element (Li) is added to all standards, blanks and unknowns in equal concentration. This element has a criteria of :

* high emission intensity.

* Is absent from biological fluid.

Applications

1- Determine the availability of alkali and alkaline earth metals which are critical for soil cultivation.

2- In agriculture, the fertilizer requirement of the soil is analyzed by flame test analysis of the soil.

3- In clinical field, Na+ and K+ ions in body fluids, muscles and heart can be determined by diluting the blood serum and aspiration into the flame.

4- Analysis of soft drinks, fruit juices and alcoholic beverages can also be analyzed by using flame photometry.

Advantages

1. Simple quantitative analytical test based on the flame analysis.
2. Inexpensive.
3. The determination of elements such as alkali and alkaline earth metals is performed easily with most reliable and convenient methods.
4. Quite quick, convenient, and selective and sensitive to even parts per million (ppm) to parts per billion (ppb) range.

FP suffer the same level of interferences as AAS from:

1- Anion due to complexation (chemical interference).

2- Matrix interference.

3- Burner interference.

4- Ionisation interference.

5- emission interference.

Limitations

- Alteration of light emission because of altered flame temp.
- It needs perfect control of flame temperature.
- Interference by other elements is not easy to be eliminated
- Heavy and transition metals , the number of absorption and emission lines is enormous and the spectra are complex
- Inadequate selectivity of WL.
- Differences in viscosity between standards and sample.

Advantages of AAS over FP

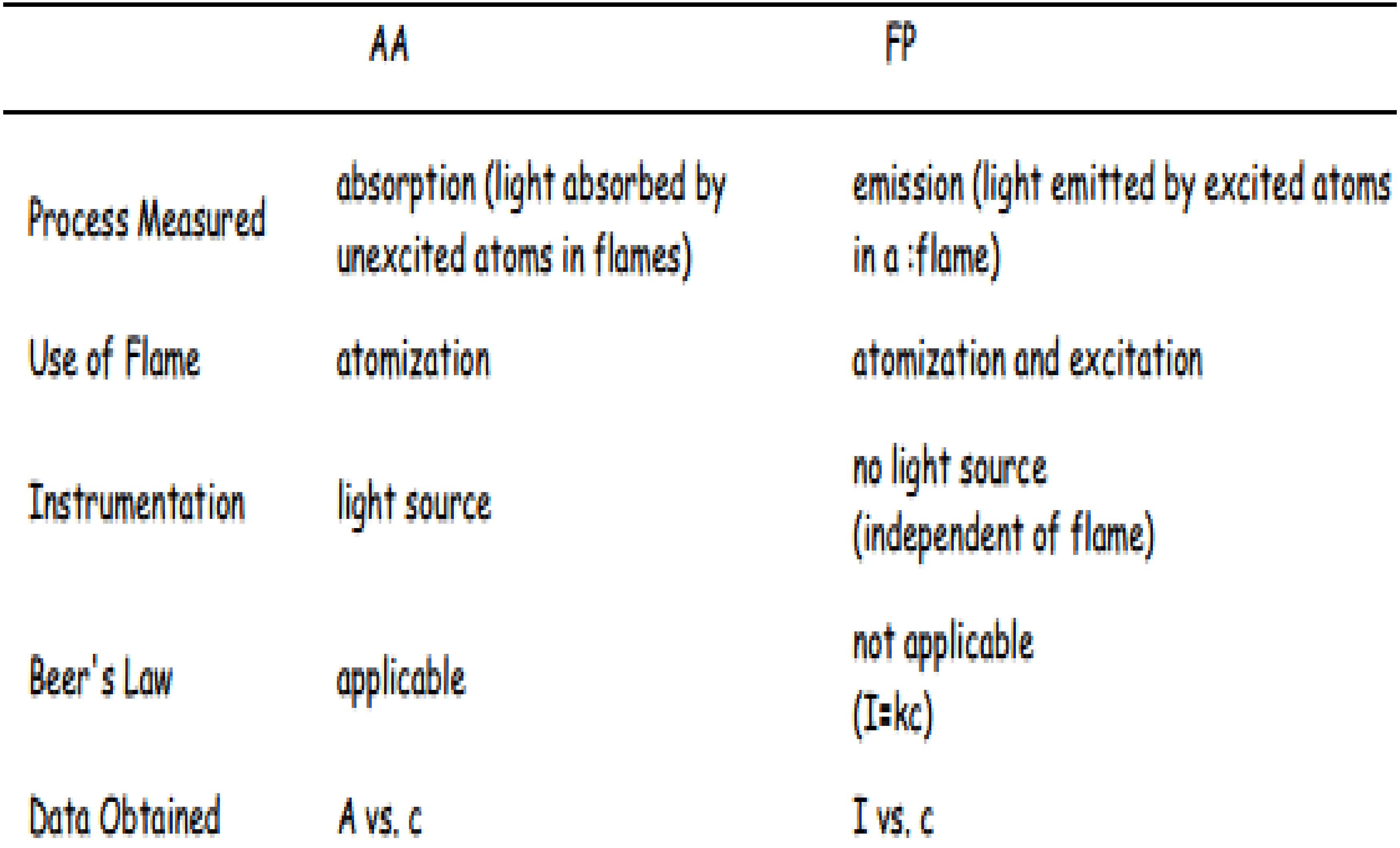
1- Sensitivity.

2- Applicability.

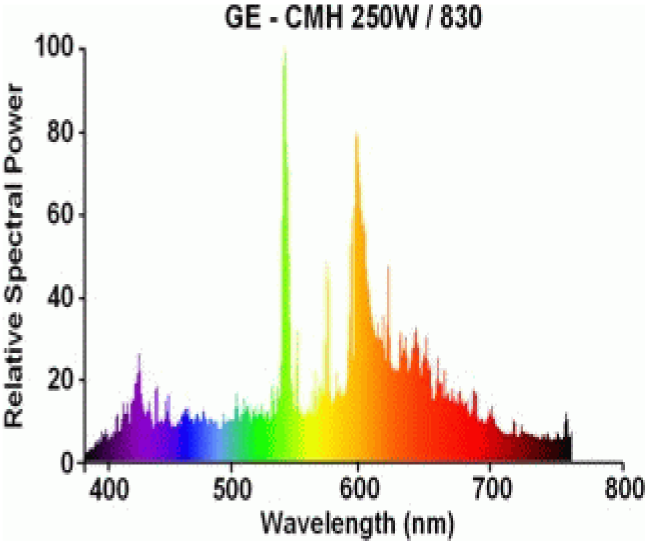
3- Smaller flame effect.

4- Less interference from other cations.

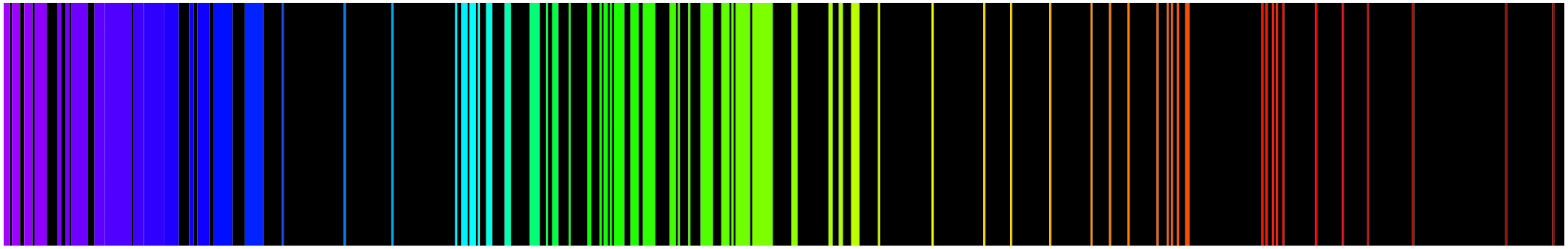
AAS Vs PF



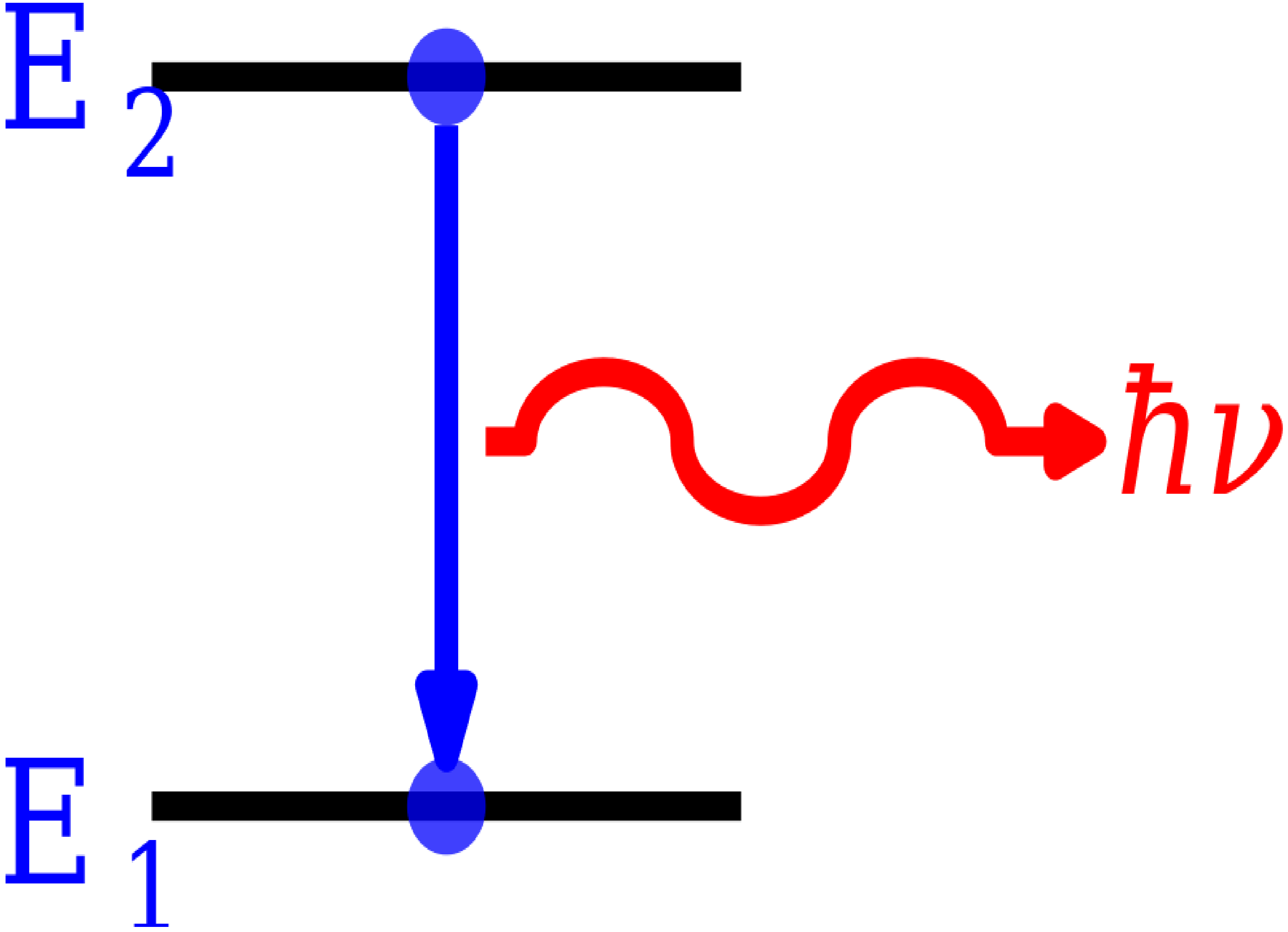
	AA	FP
Process Measured	absorption (light absorbed by unexcited atoms in flames)	emission (light emitted by excited atoms in a :flame)
Use of Flame	atomization	atomization and excitation
Instrumentation	light source	no light source (independent of flame)
Beer's Law	applicable	not applicable (I=kc)
Data Obtained	A vs. c	I vs. c



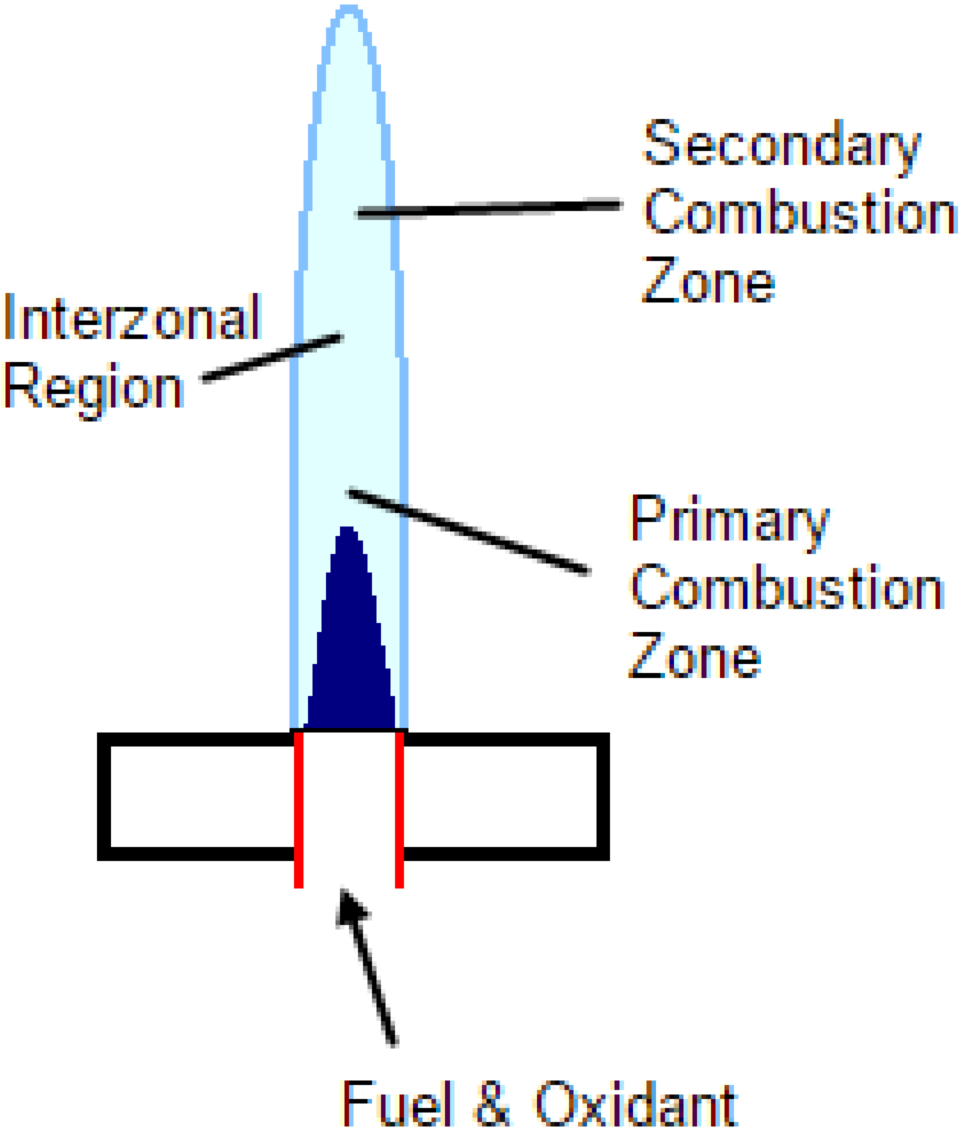
Emission spectrum of [hydrogen]



Emission spectrum of [iron]

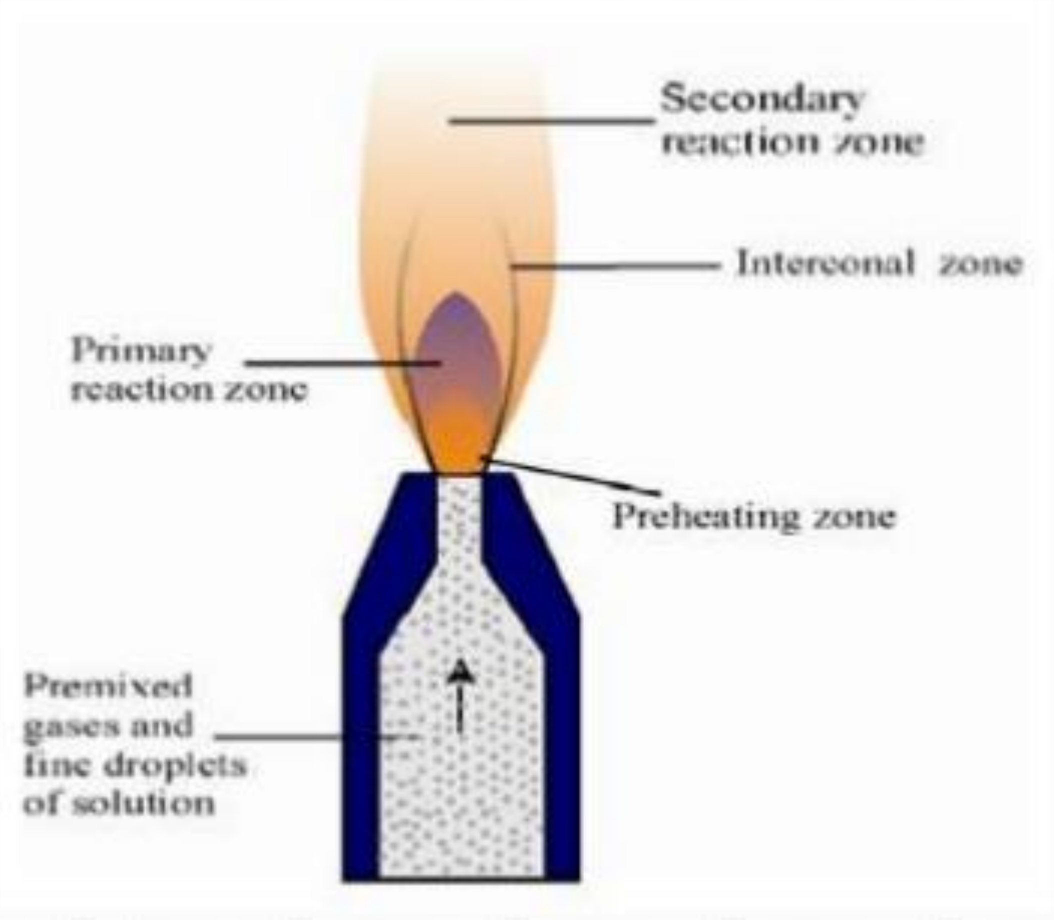


Schematic diagram of spontaneous emission


Secondary Combustion Zone
Interzonal Region
Primary Combustion Zone
Fuel & Oxidant

pg instruments

ZONES OF FLAME



REQUIREMENTS OF FLAME

- It should have proper temperature
- Temperature should remain constant throughout the operation
- There should not be any fluctuation during burning

FUNCTIONS OF FLAME

- To convert the analyte of the liquid sample into vapour state
- To decompose the analyte into atoms and simple molecules
- To excite the formed atoms/free atoms/simple molecules to emit radiant energy

BURNERS

Mecker burner

Total consumption burner

Premix of laminar flow burner

Lundergraph burner

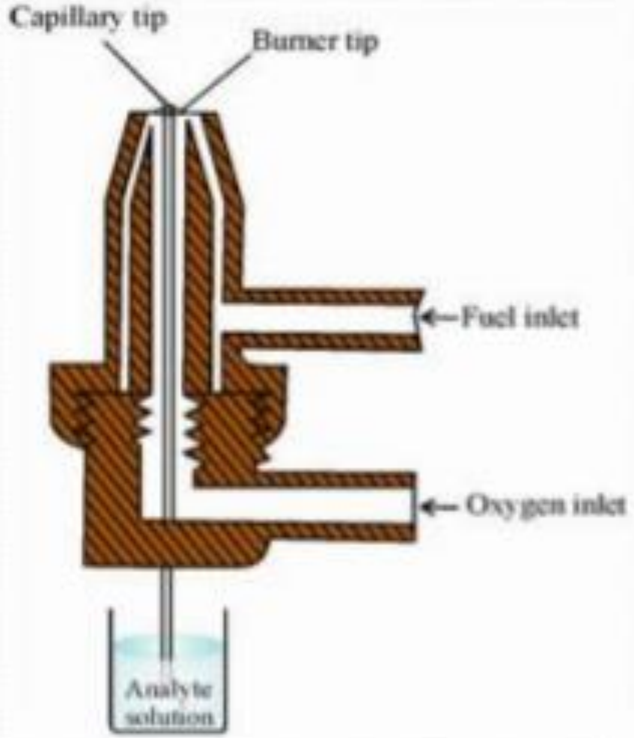
Shielded Burner

Nitrous Oxide-Acetylene Flames

MECKER BURNER

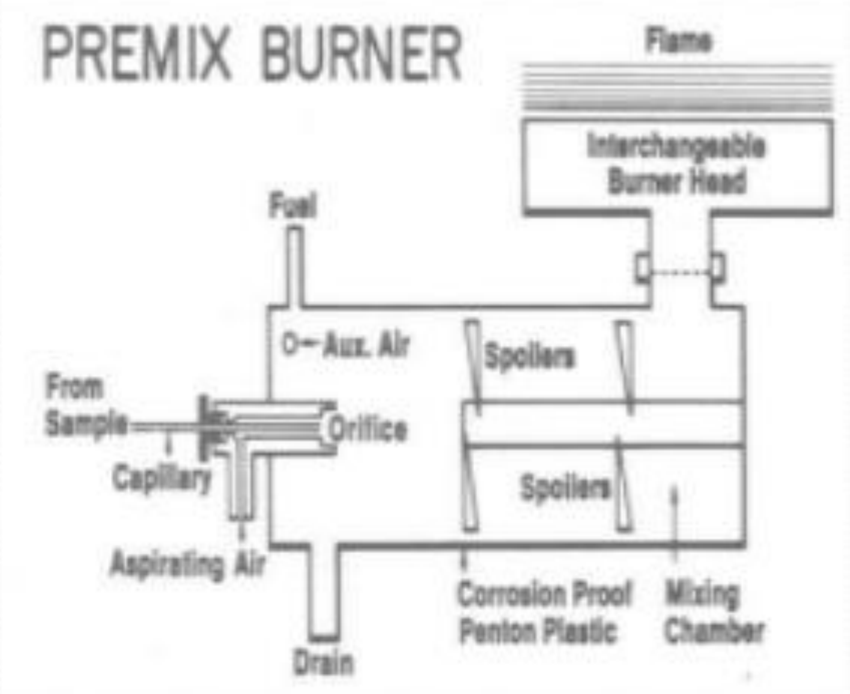
- This burner was used earlier and employed natural gas and oxygen. Produces relatively low temp. and low excitation energies. This are best used for ALKALI metals only. Now-a-days it is not used.

TOTAL CONSUMPTION BURNER



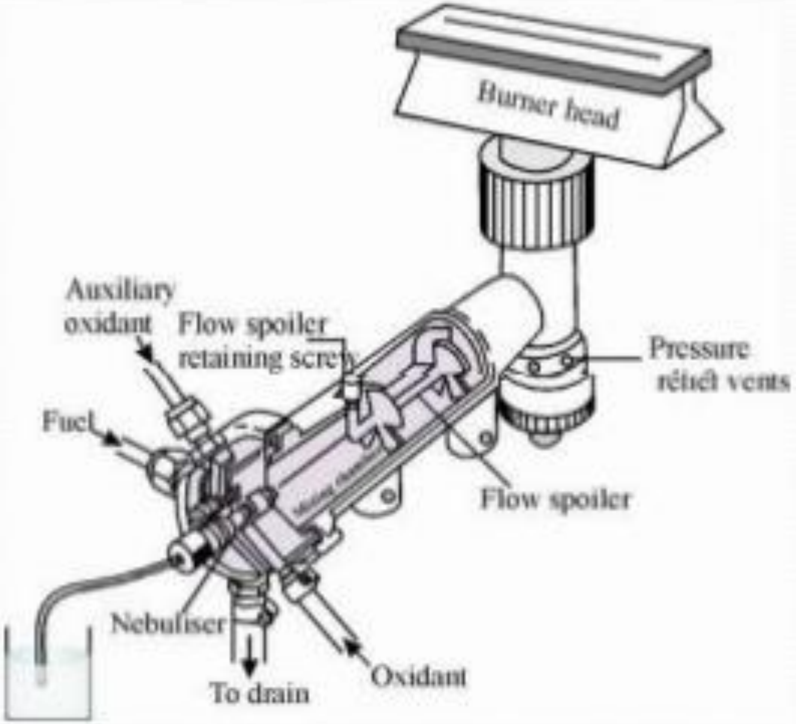
- In this burner fuel and oxidant are hydrogen and oxygen gases. Sample solution is aspirated through a capillary by high pressure of fuel and Oxidant and burnt at the tip of burner. Entire sample is consumed.

Premix OR laminar flow burner



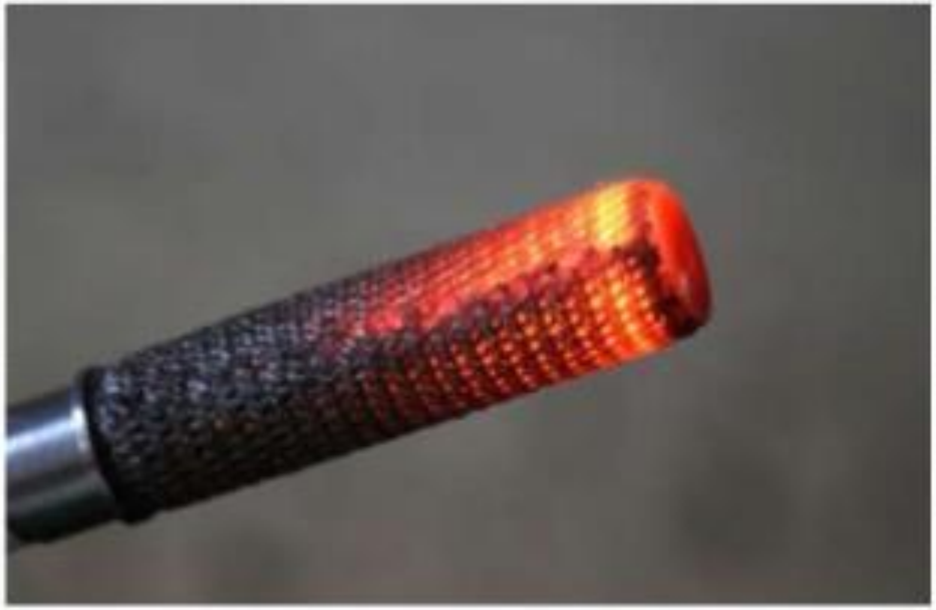
- In this type of the burner, aspirated sample, fuel and oxidant are thoroughly mixed before reaching the burner opening and then entering the flame. There is high loss of sample(95%) as large droplets are drained out.

LUNDERGRAPH BURNES



- In this sample and air is mixed in a chamber, this mixed composition is send to fuel nozzle where it is atomized. Here the sample reaches the flame is only about 5%

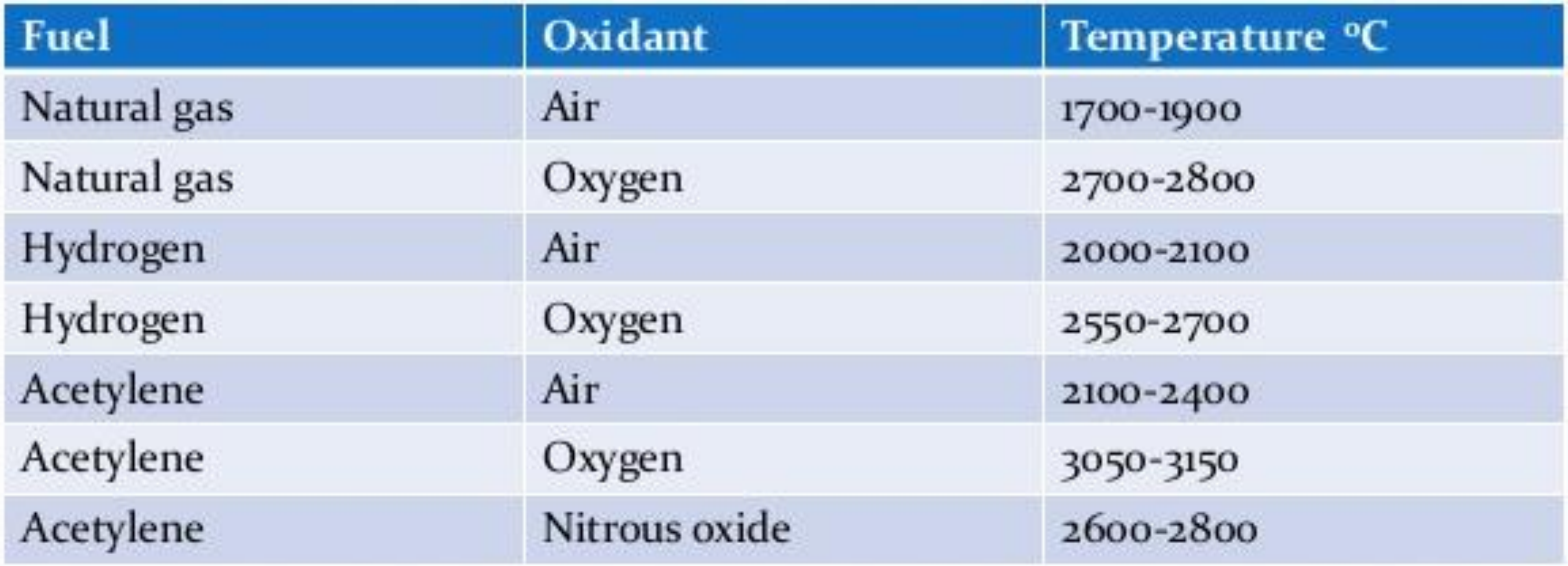
SHIELDED BURNERS



- In this flame was shielded from the ambient atmosphere by a stream of inert gas. Shielding is done to get better analytical sensitivity and quieter flame

Nitrous oxide-acetylene flame

- These flames were superior to other flames for effectively producing free atoms. The drawback of it is the high temperature reduces its usefulness for the determination of alkali metals as they are easily ionized and Intense background emission, which makes the measurement of metal emission very difficult



Fuel	Oxidant	Temperature °C
Natural gas	Air	1700-1900
Natural gas	Oxygen	2700-2800
Hydrogen	Air	2000-2100
Hydrogen	Oxygen	2550-2700
Acetylene	Air	2100-2400
Acetylene	Oxygen	3050-3150
Acetylene	Nitrous oxide	2600-2800

Interferences

- Number of factors beside the analyte affect the intensity of emitted radiation. The **analytical signals often include contributions from constituents other than analyte termed as interferences and are found to interfere the outcome of procedure.**
- 3 types:

1. **Spectral Interferences**: interference that affect spectral intensity or resolution.

   a. **1st type** of interference arises when **two elements exhibit spectra, which partially overlap,** and both emit radiation at particular wavelength. The detector cannot distinguish between the source of radiation and records the total sign, thus resulting in incorrect answer. This type of interferences are more common in high flame temperature as numerous spectral lines are produced in high temperature.

E.g., Fe line at 324.73 nm overlaps with Cu line at 324.75 nm. This Can be overcome by taking alternative wavelength with no overlap.

b. **2nd type** of spectral interference deals with **spectral lines of two or more elements which are close** but their spectra do not overlap. The filter may allow spectral lines separated by 5.0-10.0 nm to pass through, thus resulting in error in analysis. This ***can be reduced by increasing the resolution of spectral isolation system.***

c. **3rd type** of spectral interference occurs due to presence of continuous background which arises due to high concentration of salts in the sample. Some organic solvents also produce continuous background. This ***can be corrected by using suitable scanning technique.***

2. **Ionization Interference:** In certain cases, high temperature flame may cause **ionization of the metal atoms**. E.g., In case of sodium

$$Na \longrightarrow Na^+ + e^-$$

The Na+ ion possesses an emission spectrum of its own frequencies, which are different from those of Na atom. This reduces the radiant power of atomic emission. This type of interference ***can be eliminated by addition of large quantity of potassium salt to standard and sample solution.*** Potassium itself undergoes ionization due to low ionization energy and suppresses the ionization of sodium.

3. **Chemical Interferences:** This arises out of reaction between different interferents and the analyte.

a. Cation-cation interference: The presence of certain anions, such as oxalate, phosphate, sulphate and aluminate in a solution may affect the intensity of radiation emitted by an element, resulting in serious analytical error. For e.g., calcium in presence of phosphate ion forms a stable substance as $Ca_3(PO_4)_2$ which does not decompose easily, resulting in production of lesser atom. Thus calcium signal is depressed. This ***can be removed either by extraction of anion or by using calibration curve prepared from standard solutions containing same concentrations of the anion as found in the sample.***

b. Cation-cation interference: In many cases, mutual interferences of cations results in reducing element signal intensity. These interference are neither spectral nor ionic in nature and the ***actual mechanism has not been well understood***. E.g., Al interferes with Ca and Mg. Na interferes with Mg.

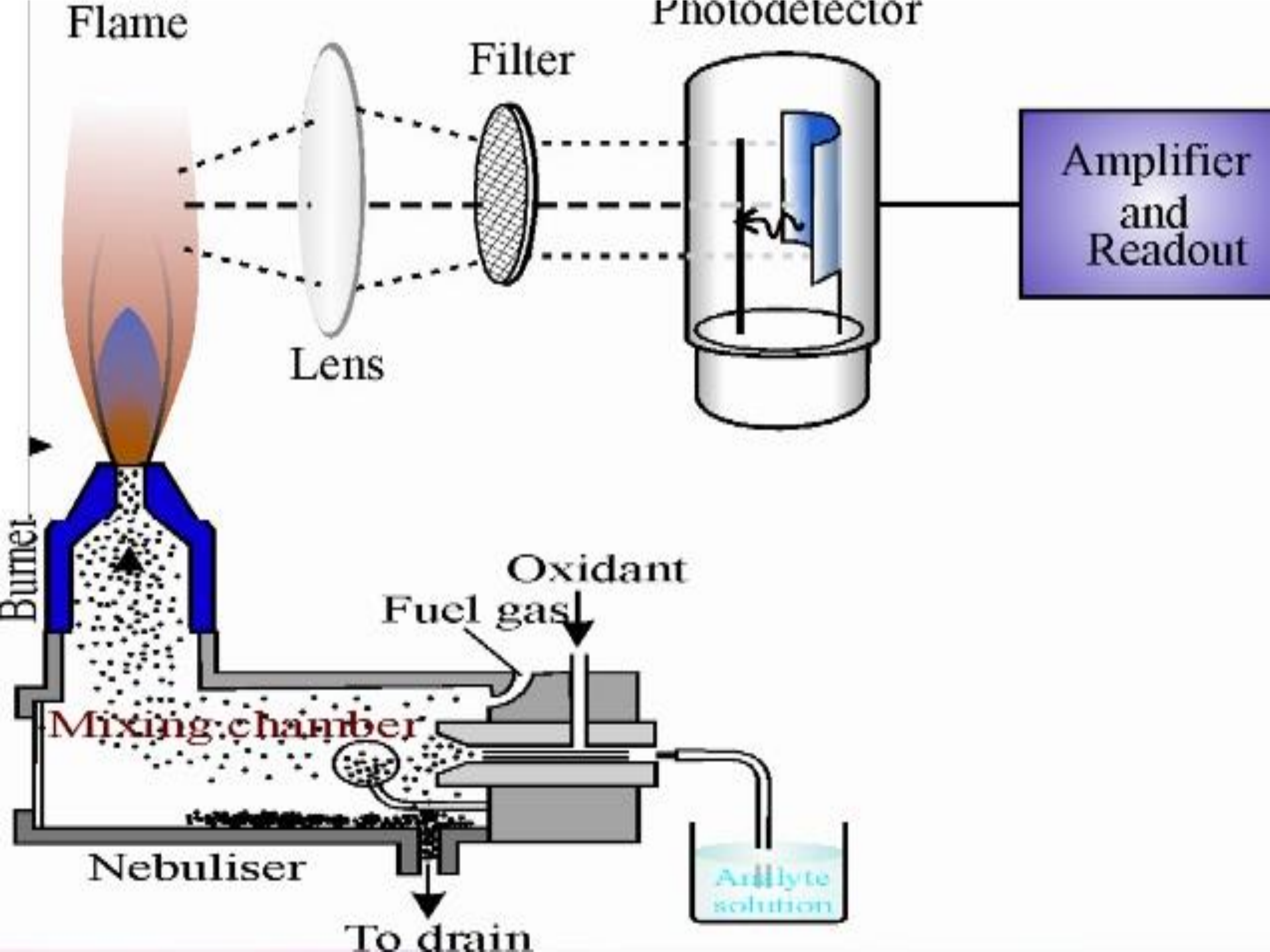
c. Oxide formation: arises due to formation of stable metal oxide if oxygen is present in flame, resulting in reduced signal intensity. E.g., Alkaline earth metal. This ***can be eliminated by either using high flame temperature to dissociate the oxides or by using oxygen-deficient environment to produce excited atom.***

Limitations

- As natural gas and air flame is employed for excitation, the temperature is not high enough to excite transition metals, therefore **the method is selective towards detection of alkali and alkaline earth metals.**
- Low temperature makes this method susceptible to certain disadvantages, most of them related to **flame stability and aspiration conditions**. *Fuel and oxidation flow rates and purity, aspiration rates, solution viscosity* affects these.
- FES is a means of determining the total metal concentration of a sample; it tells us **nothing about the molecular form of the metal** in original sample.
- **Only liquid samples** can be used.

Applications

- Flame Photometers are widely used in quality control where a **simple and quick determination of alkali or alkali earth metal is required**. They have the advantage of being significantly **lower priced** than most other atomic spectrometers.
- Biological/medical applications- **notable applications are the determinations of Na, K, Ca and Mg in body fluids and other biological samples.**
- **Food industry** – Determination of calcium and iron in beer


Flame
Photodetector
Filter
Lens
Amplifier and Readout
Burner
Oxidant
Fuel gas
Mixing chamber
Nebuliser
To drain
Analyte solution

Total Consumption Burner

In total-consumption burner, the fuel and oxidant (support) gases are mixed and combust at the tip of the burner. The fuel (usually acetylene), oxidant (usually air) and sample all meet at the base of flame. The sample is drawn up into the flame by the 'Venturi Effect', by the support gas. The gas creates a partial vacuum above the capillary barrel, causing the sample to be forced up the capillary. It is broken into a fine spray at the tip where the gases are turbulently mixed and burned. This is the usual process of 'nebulisation'.

The burner is called total consumption because the entire aspirated sample enters the flame or in other words the sample solution is directly aspirated into the flame. All desolvation, atomization, and excitation occurs in the flame.

However, the total consumption burner can be used to aspirate viscous and ‘high solids’ samples with more ease, such as undiluted serum and urine. Also, this burner can be used for most types of flames, both low- and high-burning velocity flames.

Surface mixing

Total Consumption Burner

The Venturi Effect is the reduction in fluid pressure that results when a fluid flows through a constricted section of pipe

Premix Chamber Burner

The second type of burner, most commonly used now, is the premix chamber burner, sometimes called laminar-flow chamber. Premix burners were the first purpose-designed burners, and they can be traced back more than 100 years to the Bunsen and similar laboratory burners. A premix burner system really consists of two key components, the burner head or nozzle, and the gas-air mixing device that feeds it. The fuel and support gases are mixed in a chamber before they enter the burner head (through a slot) where they combust. The sample solution is again aspirated through a capillary by the 'Venturi effect' using the support gas for the aspiration. Large droplets of the sample condense and drain out of the chamber. The remaining fine droplets mix with the gases and enter the flame. As much as 90% of the droplets condense out, leaving only 10% to enter the flame. The 90% of the sample that does not reach the flame will travels back through the mixing chamber and out as waste drain.

The premix burners are generally limited to relatively low-burning velocity flames. The most outstanding disadvantage of the premix burner is that only low burning-velocity flames can be used. A burning velocity which is higher than the rate of flow gases leaving the burner will cause the flame to travel down into the burner resulting in an explosion commonly known as flashback. Because of this limitation it is somewhat difficult to use high burning-velocity gases, which includes oxygen-based flames.

Most commercial instrument use premix burners with the option of using total-consumption burner. Premix burners are distinguished as Bunsen-, Meker-, or slot-burners according to whether they have one large hole, a number of small holes, or a slot as outlet for the gas mixture, respectively. When several parallel slots are present, they are identified as multislot burners (e.g., a three-slot burner). A popular version of premix burner is the 'Boling' burner. This is a three slot burner head that results in a broader flame and less distortion of radiation passing through at the edges of the flame. This burner warps more easily than others, though, and care must be taken not to overheat it when using organic solvents.

The difference between total-consumption burner and premix chamber burner

a) Nebulisation process

In total-consumption burner,the fuel (usually acetylene), oxidant (usually air) and sample all meet at the base of flame. The sample is drawn up into the flame by the 'Venturi Effect', by the support gas. The gas creates a partial vacuum above the capillary barrel, causing the sample to be forced up the capillary. It is broken into a fine spray at the tip where the gases are turbulently mixed and burned. This is the usual process of 'nebulisation'.

While in premix burners, the fuel and support gases are mixed in a chamber before they enters the burner head (through a slot) where they combust. The sample solution is again aspirated through a capillary by the 'Venturi effect' using the support gas for the aspiration. Large droplets of the sample condense and drain out of the chamber.

b) Size of sample droplet that enters the flame (atomization efficiency) and absorption pathlength

The total consumption burner obviously uses the entire aspirated sample, but it has a shorter path length and many larger droplets are not vaporized in the sample. The path length is extremely short, since combustion occurs only at a point above the capillary tube. Although in the total-consumption burners the entire sample is aspirated, the vaporization and atomization is poor.

Although a large portion of the aspirated sample is lost in the premix burner, the 'atomization efficiency' (efficiency of producing atomic vapour) of that portion of the sample that enters the flame is greater, because the droplets are finer. Also, the path length is longer. The sample which does reach the flame is efficiently atomized. So sensitivities are comparable with either burner in most cases.

c) Interference to flame

In total consumption burner, the larger droplets may vaporize partially, leaving solid particles in the light path. This may result in light scattering, which is registered as an absorbance. The absorbance by the sample, that is, the atomic vapour population, is generally more dependent on the gas flow rates and the height of observation in the flame than with the premix burners. The viscosity of the sample will more greatly affect the atomization efficiency (production of atomic vapour) in the total consumption burner. The resulting drops are relatively large which will cause the flame temperature to fluctuate and will scatter the source radiation. This may cause false measurements to be detected. This interference will not happen in premix burner since fine droplets of sample is produced.

d) Flame homogeneity

Total consumption burner is used in flame photometry and is not useful for atomic absorption. The reason for this is that the resulting flame is turbulent and non-homogenous because it combines the function of nebulizer and burner. Here oxidant and fuel emerge from separate ports and are mixed above the burner orifices to produce a turbulent flame. Non-homogenous flame is a property that negates its usefulness in atomic absorption, since the flame must be homogeneous, for the same reason that different sample cuvettes in molecular spectrophotometry must be closely matched. One would not want the absorption properties to change from one moment to the next because of the lack of homogeneity in the flame.

e) Noise

Combustion with the premix burners is very quiet, while with the total-consumption burner it is noisy to the detector as well as to the ear, possibly on a level similar to that of a jet engine.


* MAIN MENU *
1)ANALYSIS 2)SETUP
3)CALIBRATE 4)MISC
MICROPROCESSOR
FLAME PHOTOMETER
COMPRESSOR UNIT
EP902
FLAME PHOTOMETER

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Structure

Why use structure?

In C, there are cases where we need to store multiple attributes of an entity. It is not necessary that an entity has all the information of one type only. It can have different attributes of different data types. For example, an entity **Student** may have its name (string), roll number (int), marks (float). To store such type of information regarding an entity student, we have the following approaches:

- Construct individual arrays for storing names, roll numbers, and marks.
- Use a special data structure to store the collection of different

data types. Let's look at the first approach in detail.

```
#include<stdio.h>
void main()
{
  char names[2][10],dummy;
  int roll_numbers[2],i;
  float marks[2];
  for(i=0;i<3;i++)
  {
    printf("Enter the name, roll number, and marks of the student %d",i+1);
scanf("%s%d%f",&names[i], &roll_numbers[i],&marks[i]);
scanf("%c",&dummy);
  }
  printf("PrintingtheStudentdetails ...\n");
  for(i=0;i<3;i++)
  {
    printf("%s%d%f\n",names[i],roll_numbers[i],marks[i]);
  }
}
```

Output

```
Enter the name, roll number, and marks of the student 1Arun
90 91 Enter the name, roll number, and
marksofthestudent2Varun9156 Enter the name,rollnumber,and
marksofthestudent3Sham8969 Printing the Student details...
Arun  9091.000000
Varun 9156.000000
Sham 89 69.000000
```

What is Structure

Structureincisauser-defineddatatypethatenablesustostorethecollectionofdifferentdatatypes.Each element of a structure is called a member. Structures c a; simulate the use of classes and templates as it can store various information

The**, struct** keyword is usedtodefinethestructure.Let'sseethesyntaxtodefinethestructureinC.

Syntax

```
struct structure_name
{
   data_type
   member1;
```

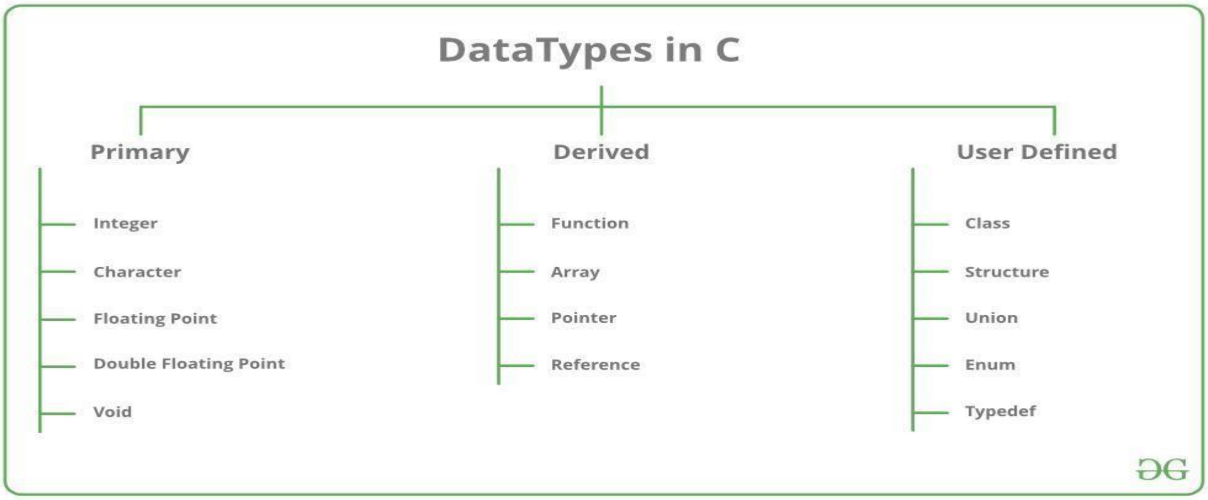
```
            data_typem
            ember2;
};
```

Data Types in C

Each variable in C has an associated data type. Each data type requires different amounts of memory and has some specific operations which can be performed over it. It specifies the type of data that the variable can store like integer, character, floating, double, etc. The data type is a collection of data with values having fixed values, meaning as well as its characteristics.

The data types in C can be classified as follows:

Types	Description
Primitive DataTypes	Arithmetic types can be further classified into integer and floating data types.
Void Types	The data type has no value or operator and it does not provide a result to its caller. But void comes under Primitive data types.
User DefinedData Types	It is mainly used to assign names to integral constants, which make a program easy to read and maintain
Derived types	The data types that are derived from the primitive or built-in datatypes are referred to as Derived Data Types.



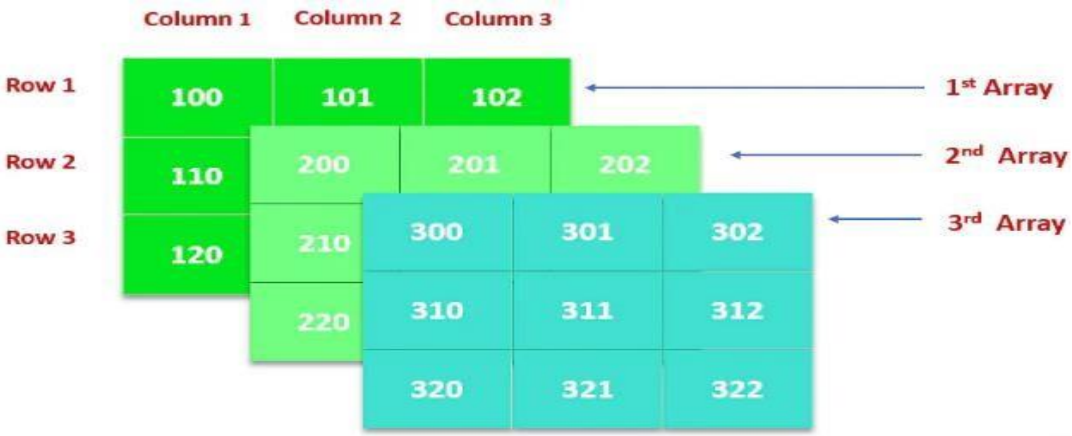
Array in C: Definition, Advantages, Declare, Initialize

Array in C can be defined as a method of clubbing multiple entities of similar type into a largergroup.
These entities or elements can be of int, float, char, or double data type or can be of user-defined data types too like structures.
In order to be stored together in a single array, all the elements should be of the same data type.
The elements are stored from left to right with the left-most index being the 0th index and the rightmost index being the (n-1) index.
Array in C are of two types; Single dimensional arrays and Multidimensional arrays.

- Single Dimensional Arrays: Single dimensional array or 1-D array is the simplest form of arrays that can be found in C. This type of array consists of elements of similar types and these elements can be accessed through their indices.

ARRAYS IN C

- Multi-dimensional Arrays: The most common type of multi-dimensional array that is used in the C language is a 2-D array. However, the number of dimensions can be more than 2 depending upon the compiler of the user's system. These arrays consist of elements that are array themselves.



Why Do We Need Arrays?

If we have a small number of elements, let us say we want 3 variables, then we can declare them separately like var1, var2, and var3. But if we have a large number of variables then we can use arrays to store them.

Let us take a real-life example. Suppose you want to make a program that prints 1-100 digits. Now in C language, you can achieve this by 2 methods. The first one is to make 100 variables and store the numbers from 1-100 in those variables separately and then print each digit. The second method is to create an array of size 100 and store the numbers in that array using a loop. These digits can be printed using a single loop in linear complexity. It is clear that the second method is more optimized and desirable than the first one as it is more convenient to store these values in a single array rather than creating 100 variables.

Declaration and Initialization of Array in C

There are various ways in which an array can be declared and initialized in various ways. You can declare an array of any data type (i.e. int, float, double, char) in C. The following ways can be used to declare and initialize an array in C.

- Array Declaration by Specifying the Size

Arrays can be declared by specifying the size or the number of array elements. The size of the array specifies the maximum number of elements that the array can hold. In the latest version of C, you can either declare an array by simply specifying the size at the time of the declaration or you can provide a user-specified size. The following syntax can be used to declare an array simply by specifying its size.

```
 // declare an array by specifying size in [].
int my_array1[20];
char my_array2[5];
// declare an array by specifying user defined size.
int size = 20;
int my_array3[size];
```

When an array is declared without allocating any value, then it stores a garbage value. If you access any uninitialized array value, then just like any uninitialized variable, it will give you a garbage value.

- **Array Declaration by Initializing Elements**

An array can be initialized at the time of its declaration. In this method of array declaration, the compiler will allocate an array of size equal to the number of the array elements. The following syntax can be used to declare and initialize an array at the same time.

```
// initialize an array at the time of declaration.
int my_array[] = {100, 200, 300, 400, 500}
```

In the above syntax, an array of 5 elements is created and even though the array size has not been specified here, the compiler will allocate a size of 5 integer elements.

- Array Declaration by Specifying the Size and Initializing Elements

An array can also be created by specifying the size and assigning array elements at the time of declaration. This method of array creation is different from the previous one. Here, if the number of initialized elements is less than the size of the array specified, then the rest of the elements will automatically be initialized to 0 by the compiler. See the following syntax to understand this.

```
// declare an array by specifying size and
// initializing at the time of declaration
int my_array1[5] = {100, 200, 300, 400, 500}; // my_array1 = {100, 200, 300, 400, 500}
//
int my_array2[5] = {100, 200, 300}; // my_array2 = {100, 200, 300, 0, 0}
```

In the above array syntax, my_array1 is an array of size 5 with all five elements initialized. Whereas, my_array2 is an array of size 5 with only three of its elements initialized. The remaining two elements of the second array will be initialized to 0 by the compiler.

- **Array Initialization Using a Loop**

An array can also be initialized using a loop. The loop iterates from 0 to (size - 1) for accessing all indices of the array starting from 0. The following syntax uses a “for loop” to initialize the array elements. This is the most common way to initialize an array in C.

```
// declare an
array.int
my_array[5];
// initialize array using a "for"
loop.int i;
for(i = 0; i < 5; i++)
{
 my_array[i] = 2 * i;
}
// my_array = {0, 2, 4, 6, 8}
```

In the above syntax, an array of size 5 is declared first. The array is then initialized using a for loop that iterates over the array starting from index 0 to (size - 1).

Access Array Elements

Since an array is stored contiguously in the memory, it has indices starting from ”0” to “array_size - 1”, also known as zero-based indexing. This indexing represents the position in the array.

The array indices are used to access any element of the array in the following way:array_name[index]

The index of the element to be accessed is specified within square brackets “[]”. The range of theindex is- integers in the range [0, size).

Examples:

```
int my_array[6];
// access 1st
element
my_array[0] =
```

```
100;
// access 4th
element
my_array[2] =
300;
// access last element
```

```
my_array[5] = 600;
```

Input and Output Array Elements

Array values can be stored by taking input from the user and storing them in the array. The following example illustrates this:

```
// input an integer element and store it
// in 1st position of the
arrayscanf("%d",
&my_array[0]);
// input a float element and store it
// in ith position of the array
scanf("%f", &my_array[i-
1]);
```

Similarly, array elements can also be displayed in the output using the printf() method. The index is specified indicating the position of the element to be printed. The following example illustratesthis:

```
// print the element stored at 1st position or 0th
indexprintf("%d", my_array[0]);
// print the element stored at ith position or (i - 1)th
indexprintf("%d", my_array[i-1]);
```

Advantages of Array in C

Arrays have a great significance in the C language. They provide several advantages to the programmers while programming. Some of them are:

- Arrays make the code more optimized and clean since we can store multiple elements in a single array at once, so we do not have to write or initialize them multiple times.
- Every element can be traversed in an array using a single loop.
- Arrays make sorting much easier. Elements can be sorted by writing a few lines of code.
- Any array element can be accessed in any order either from the front or rear in O(1) time.
- Insertion or deletion of the elements can be done in linear complexity in an array.

Disadvantages of Array in C

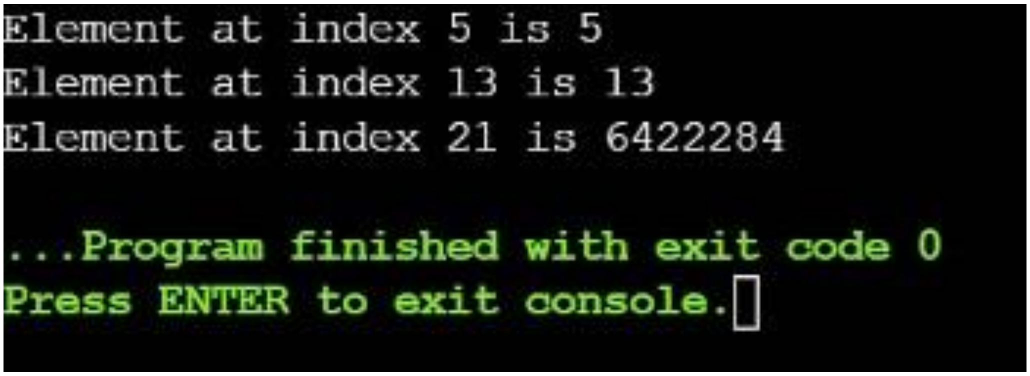
Every advantageous thing comes with some disadvantages as well. This stands true for arrays as well. Below are some of the disadvantages of the array in C:

- Accessing an array out of bounds: The first disadvantage of arrays is that they are statically allocated. This means that once their size is initialized, it can not be increased or decreased. To understand this point, consider the example given below:

```
#include
<stdio.h>int
main()
{
 //declaring the array of size 20
 int my_array[20];
 //initialising the array elements
 for (int i = 0; i < 20; i++)
 {
    //i will be the value of e
    //very ith element of the array
    my_array[i] = i;
 }
```

```
// print value at index 5 of the array
printf("Element at index 5"
       " is %d\n",
```

```
        my_array[5]);
 // Print value at index 13 of the array
 printf("Element at index 13"
        " is %d\n",
        my_array[13]);
 // Print value at index 21 of the array
 printf("Element at index 21"
        " is %d",
        my_array[21]);
 return 0;
}
```



```
Element at index 5 is 5
Element at index 13 is 13
Element at index 21 is 6422284

...Program finished with exit code 0
Press ENTER to exit console.
```

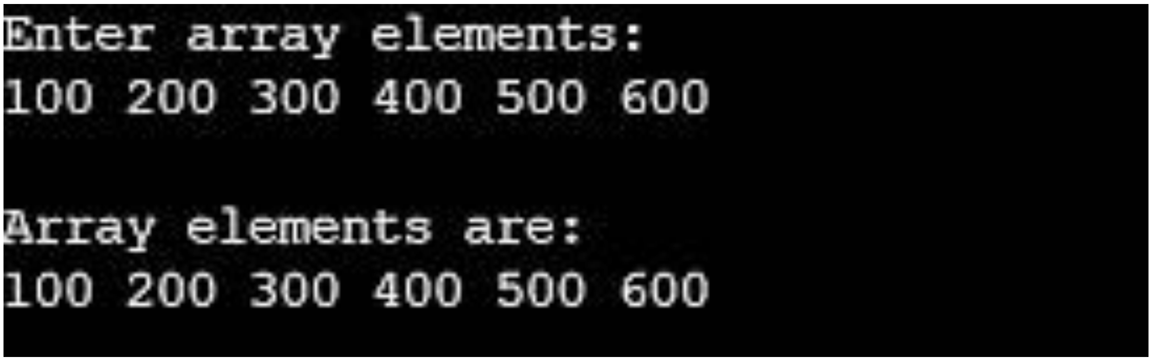
Examples of the 1-D Array in C

The following programs illustrate declaration, initialization, input/output operations, and basicoperations like insertion, deletion, sorting, and searching in the 1-D array in C.

Example 1: Array Declaration, Input, and

Output#include <stdio.h>

```
int main()
{
 // declare an array.
 int my_array[6];
 printf("Enter array elements:\n");
 // input array elements.
 int i;
 for (i = 0; i < 6; i++)
 {
    scanf("%d", &my_array[i]);
 }
 printf("\nArray elements are:\n");
 // print array elements.
 for (i=0;i<=5;i++)
 {
    printf("%d ", my_array[i]);
 }
 return 0;
}
```



```
Enter array elements:
100 200 300 400 500 600

Array elements are:
100 200 300 400 500 600
```

Strings

Strings are used for storing text/characters.
For example, "Hello World" is a string of characters.
Create an array of characters to make a string in C:

The string can be defined as the one-dimensional array of characters terminated by a null ('\0'). The character array or the string is used to manipulate text such as word or sentences. Each character in the array occupies one byte of memory, and the last character must always be 0. The termination character ('\0') is important in a string since it is the only way to identify where the string ends. When we define a string as char s[10], the character s[10] is implicitly initialized with the null in the memory.

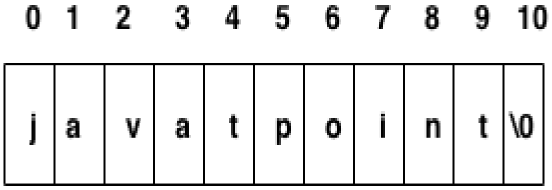
There are two ways to declare a string in c language.

1. By char array
2. By string literal

Let's see the example of declaring **string by char array** in C language.

1. **char** ch[10]={'j', 'a', 'v', 'a', 't', 'p', 'o', 'i', 'n', 't', '\0'};

As we know, array index starts from 0, so it will be represented as in the figure given below.



0	1	2	3	4	5	6	7	8	9	10
j	a	v	a	t	p	o	i	n	t	\0

we can write the above code as given below:

1. **char** ch[]={'j', 'a', 'v', 'a', 't', 'p', 'o', 'i', 'n', 't', '\0'};

We can also define the **string by the string literal** in C language. For example:

1. **char** ch[]="javatpoint";

In such case, '\0' will be appended at the end of the string by the compiler.**There are two ways to traverse a string.**

- By using the length of string
- By using the null character.

Let's discuss each one of them.

Using the length of string

Let's see an example of counting the number of vowels in a string.

```
#include<stdio.h>
void main ()

{
   char s[11] = "javatpoint";
   int i = 0;
   int count = 0;
   while(i<11)
   {
      if(s[i]=='a' || s[i] == 'e' || s[i] == 'i' || s[i] == 'u' || s[i] == 'o')
      {
         count ++;
      }
      i++;

   }
   printf("The number of vowels %d",count);
}
```

Output

```
The number of vowels 4
```

Using the null character

Let's see the same example of counting the number of vowels by using the null character.

```
#include<stdio.h>
void main ()
{
   char s[11] = "javatpoint";
   int i = 0;
   int count = 0;
   while(s[i] != NULL)
   {
      if(s[i]=='a' || s[i] == 'e' || s[i] == 'i' || s[i] == 'u' || s[i] == 'o')
      {
         count ++;
      }
          i++;
   }
   printf("The number of vowels %d",count);

}
```

Output

```
The number of vowels 4
```

Accepting string as the input

Till now, we have used scanf to accept the input from the user. However, it can also be used in the case of strings but with a different scenario. Consider the below code which stores the string while space is encountered.

```
#include<stdio.h>
```

```
void main ()
{
   char s[20];
   printf("Enter the string?");
   scanf("%s",s);
   printf("You entered %s",s);
}
```

Output

```
Enter the string?javatpoint is the
bestYou entered javatpoint
```

It is clear from the output that, the above code will not work for space separated strings.

Here we must also notice that we do not need to use address of (&) operator in scanf to store a string since string s is an array of characters and the name of the array, i.e., s indicates the base address of the string (character array) therefore we need not use & with it.

C String Functions

There are many important string functions defined in "string.h" library.

No.	Function	Description
1)	strlen(string_name)	returns the length of string name.
2)	strcpy(destination, source)	copies the contents of source string to destination string.
3)	strcat(first_string, second_string)	concats or joins first string with second string. The result of the string is stored in first string.
4)	strcmp(first_string, second_string)	compares the first string with second string. If both strings are same, it returns 0.
5)	strrev(string)	returns reverse string.
6)	strlwr(string)	returns string characters in lowercase.
7)	strupr(string)	returns string characters in uppercase.

```
#include<stdio.h>

#include <string.h>

int main()

{

char ch[20]={'j', 'a', 'v', 'a', 't', 'p', 'o', 'i', 'n', 't', '\0'};

  printf("Length of string is: %d",strlen(ch));

 return 0;

}
```

Program to demonstrate String built in function

```
#include<stdio.h
>
#include<conio.
h>void main(){
char
string1[25],string2[25];int
l;
printf("***** performing string length
******\n");printf("enter only one string \n");
scanf("%s",string1);
l = strlen(string1);
printf("the string length is %d\n\n",l);
printf("**** performing string concatenation ****\n");
printf("enter two strings\n");scanf("%s%s",string1,string2);
printf("the concatenated string is
%s\n\n",strcat(string1,string2));printf("***** performing
string compare *****\n"); printf("enter two strings \n");
scanf("%s%s",string1,string2)
; if(strcmp(string1,string2) =
= 0)printf("strings are
equal\n");elseprintf("strings
are not equal\n");
printf("*** performing string copy ****\n");
printf("enter the two strings\n");scanf("%d%d",string1,string2);
printf("the first string is %s and second string is
%s\n",string1,string2);strcpy(string1,string2);
printf("the first string is %s and second string is %s\n",string1,string2);
}
```

Character Handling Functions in C

Character functions need ctype.h header file to be included in the program. Different characterfunctions provided by C Language are:

1. isalpha():
   This function checks whether the character variable/constant contains alphabet or not.
2. isdigit()
   This function checks whether the character variable/ constant contains digit or not.
3. isalnum()
   This function checks whether the character variable/constant contains an alphabet or digit.
4. ispunct()
   This function checks whether the character variable/constant contains a punctuator or not. Punctuators are comma, semicolon etc.
5. isspace()
   This function checks whether the character variable/constant contains a space or not.

Program to demonstrate the use of character functions.

```
#include<ctype.h>
#include<stdio.h>
int main()
{
char n;
printf("\nEnter a character=");
n=getche();
if(isalpha(n))
printf("\nYou typed an alphabet");
if(isdigit(n))
printf("\nYou typed a digit");
if(isalnum(n))
printf("\nYou typed an alphabet or digit");
if(isspace(n))
printf("\nYou typed a blank space");
if(ispunct(n))
printf("\nYou typed punctuator");
return(0);
}
```

Output

```
Enter a character=A
You typed an alphabet
```

6. isupper()
   This function checks whether the character variable/constant contains a capital letter alphabet ornot.
7. islower()
   This function checks whether the character variable/constant contains a lowercase alphabet ornot.
8. toupper()

This function convert’s lowercase alphabet into uppercase alphabet.

9. tolower()

This function converts an uppercase alphabet into lowercase alphabet.

Program to use of islower,isupper,tolower(),toupper().

```
#include<ctype.h>
#include<stdio.h>        int
main()
{
char n;
printf("\nEnter an alphabet=");
n=getche();
if(islower(n))
n=toupper(ch); else
ch=tolower(ch);
printf("\nNow alphabet=%c",n);
return(0);
}
```

Output

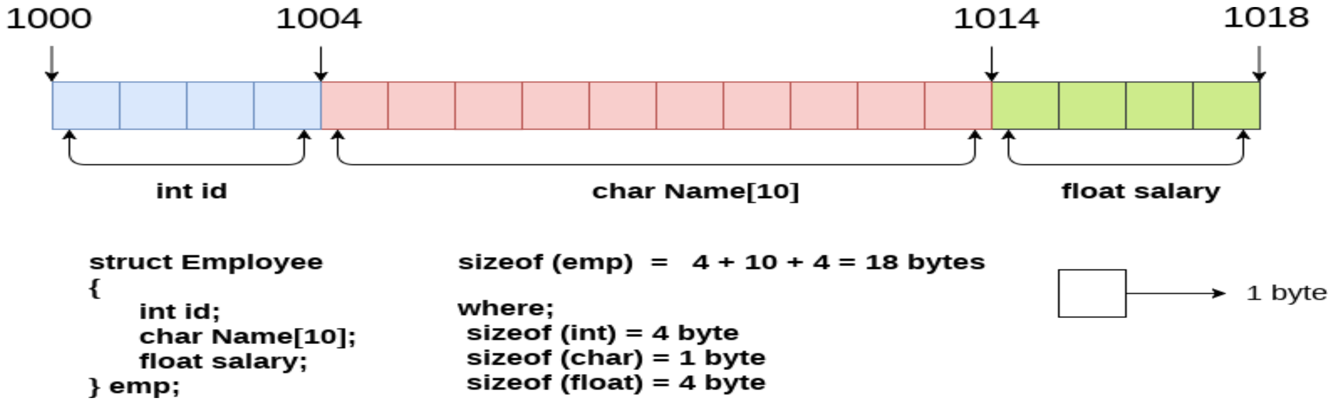
```
Enter an alphabet=A
```

```
    .
    .
    data_typememeberN;
};
```

Let'sseetheexampletodefineastructureforanentityemployeeinc.

```
structemployee
{
    intid;
    charname[20];
    floatsalary;
};
```

The following image shows the memory allocation of the structure employee that is defined in the above example.

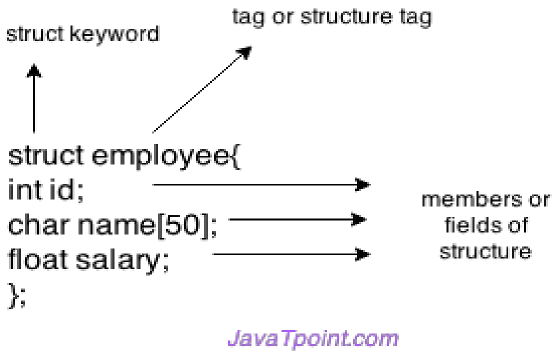


```
struct Employee
{
    int id;
    char Name[10];
    float salary;
} emp;
```

```
sizeof (emp)  =  4 + 10 + 4 = 18 bytes

where;
 sizeof (int) = 4 byte
 sizeof (char) = 1 byte
 sizeof (float) = 4 byte
```

Here,**struct**isthekeyword;**employee**isthename ofthestructure;**id**,**name**,and**salary**arethe members or fields of the structure. Let's understand it by the diagram given below:



```
struct employee{
int id;
char name[50];
float salary;
};
```

Declaringstructurevariable

Wecandeclareavariableforthestructuresothatwecanaccessthememberofthestructureeasily.There are two ways to declare structure variable:

1. Bystructkeywordwithinmain()function
2. Bydeclaringavariableatthetimeofdefiningthestructure.

1st way:

Let'sseethe exampletodeclarethestructurevariablebystructkeyword.Itshouldbedeclaredwithinthe main function.

```
structemployee

{int id;

charname[50];

floatsalary;

};
```

Nowwritegivencodeinsidethemain() function.

structemployeee1,e2;

Thevariablese1ande2canbeusedtoaccessthevaluesstoredinthestructure

2ndway:

Let'sseeanotherwaytodeclarevariableatthetimeofdefiningthestructure.

```
structemployee
{int id;
charname[50];
floatsalary;
}e1,e2;
```

Which approach isgood

Ifnumberofvariablesisnotfixed,usethe1stapproach.Itprovidesyoutheflexibilitytodeclarethe structure variable many times.

Ifno.ofvariables arefixed,use2ndapproach.Itsavesyourcodetodeclareavariableinmain()function.

Accessingmembersofthestructure

Therearewaystoaccessstructuremembers: By.

(member or dot operator)

1.p1.id

CStructureexample

Let'sseeasimpleexampleofstructureinC language. #include<stdio.h>

```
#include<string.h>
structemployee
{
intid;
charname[50];
}e1;//declaringe1variableforstructure
intmain()
{
//storefirstemployeeinformation
e1.id=101;
strcpy(e1.name,"SonooJaiswal");//copyingstringintochararray
//printingfirstemployee information
```

```
printf( "employee 1 id : %d\n",
e1.id);printf("employee1name:%s\n",e1.na
me); return 0;
}
```

Output:

```
employee1id:101
employee1 name:Sonoo Jaiswal
```

Let'sseeanotherexampleofthestructurein [Clanguage]()tostore manyemployeesinformation. #include<stdio.h>

```
#include<string.h>
structemployee
{int id;
charname[50];
floatsalary;
}e1,e2;//declaringe1ande2variables forstructure
intmain()
{
//storefirstemployeeinformation
e1.id=101;
strcpy(e1.name,"SonooJaiswal");//copyingstringintochararray
e1.salary=56000;
//storesecondemployeeinformation e2.id=102;
strcpy(e2.name,"JamesBond");
e2.salary=126000;
//printing first employee information
printf("employee1id:%d\n",e1.id);
printf( "employee 1 name : %s\n", e1.name);
printf("employee1salary:%f\n",e1.salary);
//printing second employee information
printf( "employee 2 id : %d\n",
e2.id);printf("employee2name:%s\n",e2.na
me);
printf("employee2salary:%f\n", e2.salary);
return0;
}
```

Output:

```
employee1id:101
employee 1 name : Sonoo Jaiswal
employee1salary:56000.000000
employee2id:102
employee 2 name : James Bond
employee2salary:126000.000000
```