ENGINEERING CHEMISTRY GR22A1005

Course Objectives:

- To relate how the basic concepts and principles of chemistry can be applied to practical utility in a broader perspective of the society.

- To distinguish the ranges of electromagnetic spectrum and its interaction with matter and to develop knowledge of various spectroscopic techniques at atomic and molecular levels.

- To identify and apply various principles of electrochemistry, corrosion and water treatment which are essential for an engineer in industry

- To acquire knowledge of existence of different organic molecules in different stereochemical useful for understanding reaction path ways.

- To bring adaptability to the concepts of chemistry and to acquire the required skills to become a perfect engineer.

Course Outcomes:

- Analyze microscopic chemistry in terms of atomic and molecular orbitals and intermolecular forces.

- Relate electromagnetic spectra used for exciting different molecular energy levels in various spectroscopic techniques and their application in medicine and other fields.

- Understand the fundamental principles of electrochemistry for energy production and corrosion prevention.

- Recognise various problems related to corrosion in industry and is able to explain different prevention techniques.

- Know the origin of different types of engineering materials used in modern technology and Interpret different problems involved in industrial utilization of water.

Unit-1 Atomic and Molecular Structure

- Atomic and molecular orbitals

- Linear Combination of Atomic Orbitals (LCAO)

- Molecular orbitals of homo-nuclear diatomic molecules

- MO energy diagrams of N_2, and O_2.

- Metallic bonding

- Valence Bond Theory

- Crystal Field Theory

- Crystal Field Splitting of transition metal ion d-orbitals in tetrahedral

- Octahedral and square planar geometries.

Unit-II: Spectroscopic Techniques & Applications

Contents

- Regions of electromagnetic spectrum, Molecular spectroscopy

- Rotational Spectroscopy: Rotation of molecules, rotational spectra of rigid diatomic molecules , selection rules.

- Vibrational Spectroscopy: The vibrating diatomic molecule, simple and anharmonic oscillators of a diatomic molecule, selection rules, applications of IR spectroscopy.

- Nuclear Magnetic Resonance:Criteria for NMR activity (Magnetic and non-magnetic nuclei), Basic concepts and Principle of 1H NMR spectroscopy, Chemical shift- Shielding and Deshielding. Magnetic Resonance Imaging.

Unit III: Batteries and Corrosion

• Batteries: Primary and Secondary types, Lithium ion and Lead acid batteries. Fuel cells: Definition, Hydrogen-Oxygen fuel cell and Microbial Fuel cell – working principle and applications.

• Corrosion: Definition, causes and effects of corrosion, Theories of chemical and electro chemical corrosion with mechanism, Differential metal corrosion - Galvanic corrosion, Differential aeration corrosion - pitting corrosion, Factors affecting corrosion – Nature of metal (Position of metal, Relative areas, Purity and Passivity), Nature of Environment (pH, Temperature and Humidity), Corrosion control methods: Cathodic protection (sacrificial anodic and impressed current cathodic protection), Metallic coatings: Hot dipping- galvanization and tinning.

Unit IV: Engineering Materials and Water Technology

• Semiconductors: Si and Ge - preparation, purification and crystal growth by zone refining and Czochralski pulling methods, Doping – Epitaxy, Diffusion and Ion implantation.

• Plastics: Comparison between thermoplastics and thermosets, Fabrication of plastics - compression moulding and injection moulding. Conducting polymers – Definition, classification and applications.

• Water: Hardness - Causes, types and units. Boiler troubles-scales and sludges, caustic embrittlement. Water purification: Demineralization by Ion-exchange process, Desalination by reverse osmosis method.

Unit V: Stereochemistry and Energy Resources

• Stereochemistry: Elements of symmetry-plane of symmetry, centre of symmetry, alternating axis of symmetry. Chirality, Enantiomers – tartaric acid, Diastereomers-2,3-dichloropentane, Conformational analysis of n-butane. Structure, synthesis and pharmaceutical applications of aspirin and ibuprofen.

• Energy sources: Fossil Fuels: Coal –types, analysis of coal- proximate and ultimate analysis and their significance, Petroleum-its composition, Cracking – Definition, Fluid bed catalytic cracking, Knocking and its mechanism in Internal Combustion engine, Octane rating, Hydrogen gas generation by Electrolysis process.

Gokaraju Rangaraju Institute of Engineering & Technology
(Autonomous)
Bachupally, Kukatpally, Hyderabad

Engineering Chemistry
Unit-I : Atomic & Molecular Structure

Lesson-1
Atomic & Molecular orbitals

M.Haritha Kiranmai,Faculty of Chemistry
Dept.of Humanities & Sciences
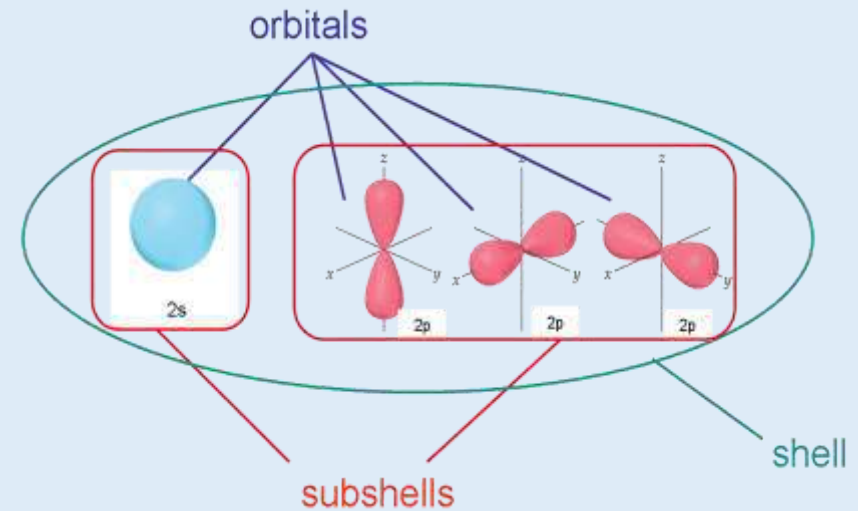
*Few slides & pictures are taken from different websites

Topics to be discussed

➢Atomic orbitals

➢Molecular orbitals

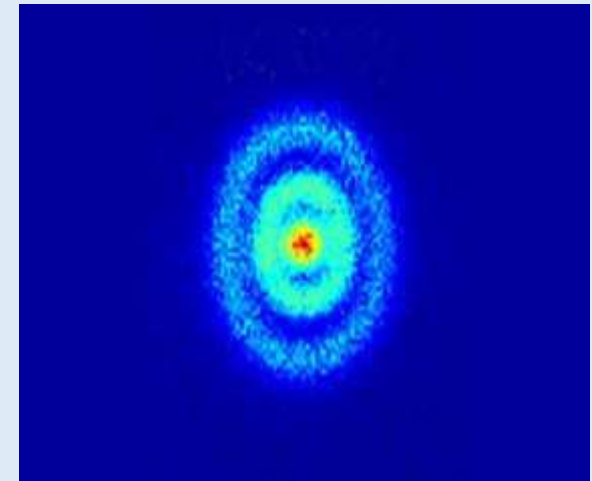Orbit: a fixed circular path describes the moving electron around a nucleus. Also called as energy level/shell.
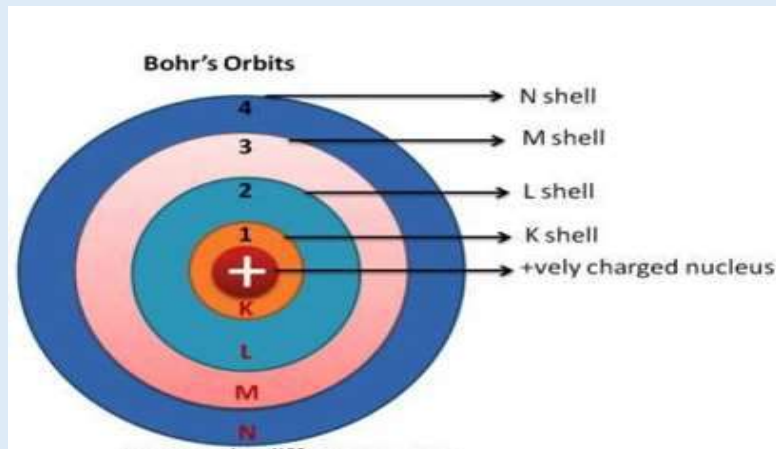
Orbital : the space around nucleus where there is probability of finding an electron is maximum

- **Atomic Orbital**

Atomic orbitals are defined as three-dimensional region (or space) around the nucleus where there is higher probability of finding an electron of specific energy.

Orbit	Orbital
Fixed circular path describes the moving electron around a nucleus	3-D in space around nucleus where there is probability of finding an electron is maximum
2-D representation	3-D representation
Position & velocity of a moving electron can be calculated with great accuracy	Can be determined with in limits of Heisenberg Uncertainty principle
Distance of the orbit from the nucleus for a given electron is fixed	Impossible to know the exact position of an electron
Movement of electron is known definitely	only probability of finding electron
Maximum capacity of an orbit is $2n^2$	Can accommodate only 2 electrons
All orbits are circular	Different shapes
Do not have directional properties	Except S, all have directional properties

Quantum Mechanics / wave mechanics:

Examines the motion of Objects

Atomic Orbitals

- specified by three quantum numbers

Quantum Mechanics: The branch of Science which takes into consideration De Broglie concepts of dual nature of matter & Plank's quantum theory & is able to explain the phenomena related to small particles is known as Quantum Mechanics.

Classical Mechanics	Quantum Mechanics
1. Deals with macroscopic objects.	1. Deals with microscopic particles.
2. Based on Newton's Laws of Motion.	2. Based on Heisenberg uncertainty principle & de Broglie's dual nature of matter.
3. Maxwell's Electromagnetic Wave Theory according to which, any amount of energy maybe emitted (or) absorbed continuously.	3. Planck's Quantum Theory- only discrete values of energy are emitted (or) absorbed.
4. The state of the system is defined by specifying all the forces acting on particles as well as their positions and velocities.	4. It gives probabilities of finding particles at various locations in space.

Reflection spot

Mention the four quantum numbers.

Principal quantum number
Azimuthal quantum number
Magnetic quantum number
Spin quantum number

Quantum numbers

- Values which are used to describe the energy levels of atoms and molecules(n,l,m,s)

- Arise as a natural consequence of the solution of Schrodinger wave equation.

- According to Heisenberg uncertainty principle it is not possible to give exact position of an electron and its energy at the same time.

- But the probability of finding an electron in an orbital of given energy can be determined.

électron

Noyau
Proton
Neutron
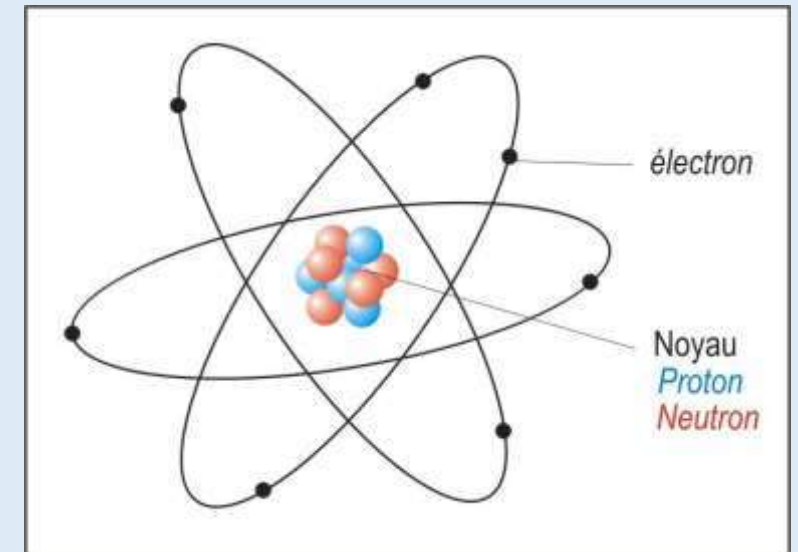
Schrodinger Wave Equation

In terms of cartesian co-ordinates

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{8\pi 2 m}{h2}(E - V)\psi = 0$$

Represents the wave motion of particle in three dimensions

m- mass of the particle

V- potential energy

E – total energy

x,y,z – coordinates of particle

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}+\frac{8\pi^2m}{h^2}(E-V)\psi=0$$

In terms of spherical coordinates
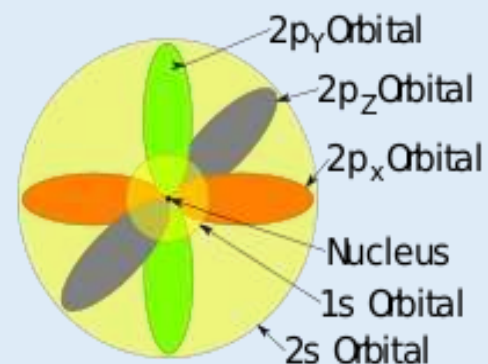r – radial coordinate
Θ,φ – angular coordinates

$(r,\phi,\theta,)$ or (x,y,z)

$r^2=x^2+y^2+z^2$

$x=r\sin\theta\cos\phi$

$y=r\sin\theta\sin\phi$

$z=r\cos\theta$
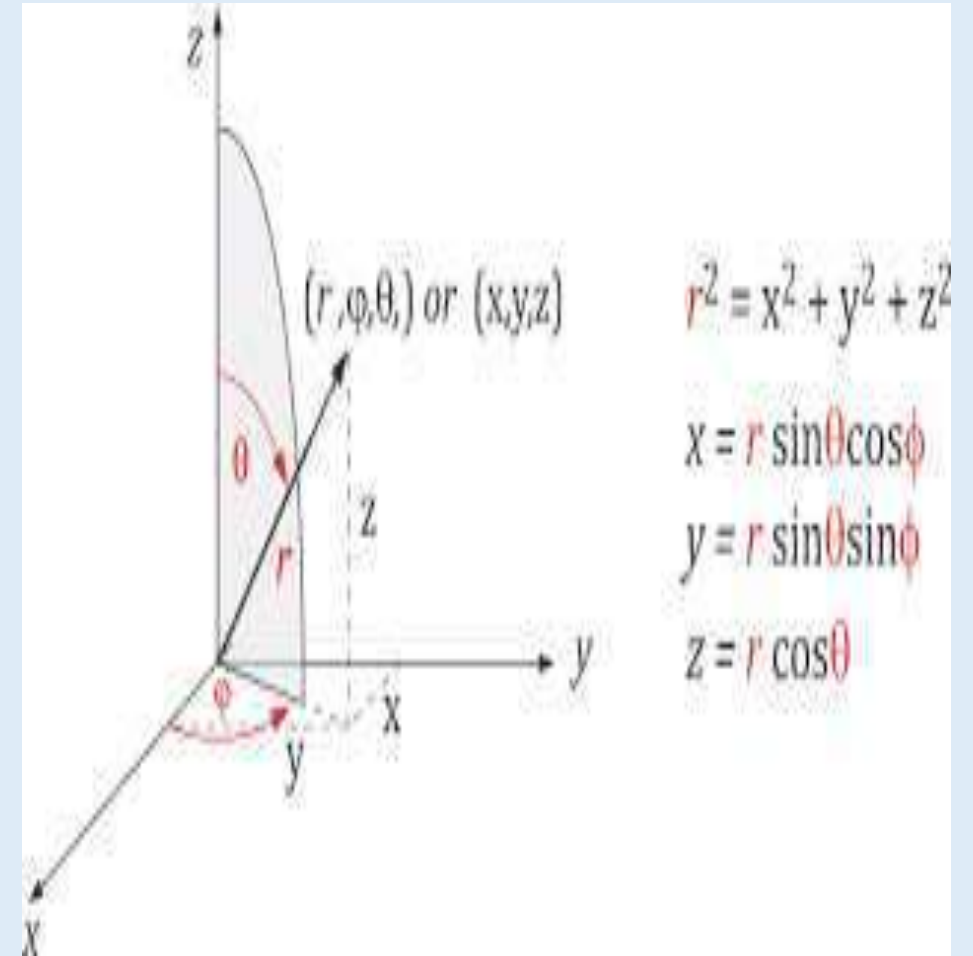
- The Solutions of Schrodinger wave equation obtained in terms of expression for R, θ & φ are acceptable solutions only if they follow the following restriction of n, l & m.

- Principal quantum number (n) = 1,2,3…………

- Azimuthal Quantum Number (l) = 0,1,2, …(n-1)

- Magnetic Quantum Number (m) = 0,1, 2, n±1, ±2, ……±l (or –l to +l)

- The quantum mechanical approach helps us to calculate the value of 'Ψ' for an electron of known values of n , l & m.

- 'Ψ' is wave function ,$Ψ^2$ is probability of finding an electron at a point.

- Depending on the values of 'l' the orbitals or electrons are given.

➢l=0 – s-orbital, electrons are in s-orbital electrons

➢l=1 – p-orbital

➢l=2 – d-orbital

➢l=3 – f-orbital

Quantum Numbers

Quantum Number	Symbol	Range	Importance
Principal Quantum Number	n	$n=1,2,3,4\ldots$	Relative size and energy level of an orbital
Azimuthal Quantum Number	l	$l=0,1,2,3,4$ (0 to n-1)	Shape of the orbital
Magnetic Quantum Number	m_l	$m_l= +l$ to $-l$	Orientation of orbital in space

Shell n	Subshell l	Subshell Notation	Orientation m	Number of Orbitals
1	0	1s	0	1
2	0	2s	0	1
	1	2p	-1 0 +1	3
3	0	3s	0	1
	1	3p	-1 0 +1	3
	2	3d	-2 -1 0 +1 +2	5
4	0	4s	0	1
	1	4p	-1 0 +1	3
	2	4d	-2 -1 0 +1 +2	5
	3	4f	-3 -2 -1 0 +1 +2 +3	7

2p$_Y$ Orbital
2p$_Z$ Orbital
2p$_X$ Orbital
Nucleus
1s Orbital
2s Orbital

Shapes of Orbitals

The Shape of the orbital can be found from the probabilities of different points around the nucleus, which are obtained by finding the values of the Wave function $\Psi(r,\theta,\phi)$.

Reflection spot

What are the shapes of different orbitals?

Shapes of Orbitals

The First Four Atomic Orbitals: s, p, d, f

Orbital Type — **Spatial Orientations**
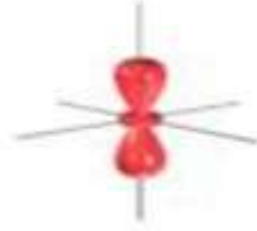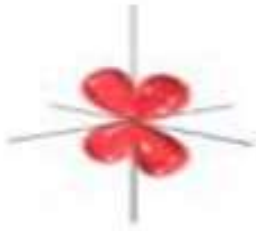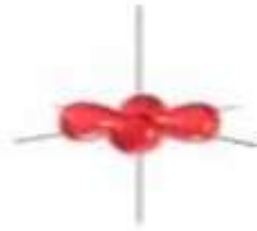
s
The s orbital has only one shape, which is spherical.
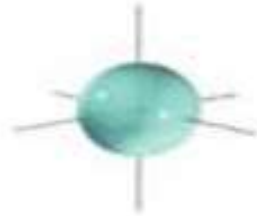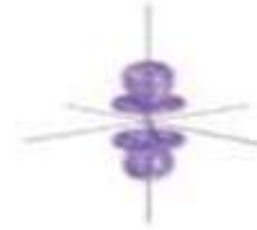
p
There are three p orbitals. They differ by orientation.
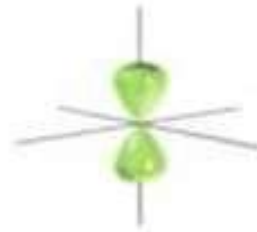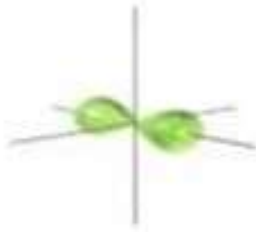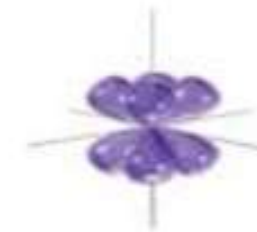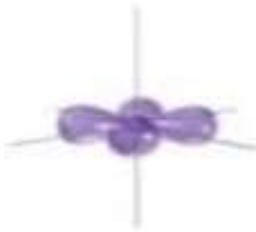
d
There are five d orbitals.

f
There are seven f orbitals.

Molecular Orbitals

- It is the region around the nuclei of the bonded atoms in a molecule where the probability of finding an electron is maximum

- Types Of MO's: Greek letters

- σ (sigma symmetry) – σ, σ*

- π (pi symmetry)- π, π*

- δ (delta symmetry)- δ, δ*

- ϕ (phi symmetry)- ϕ, ϕ*

- γ (gamma symmetry) - γ, γ*

Differences between…..

Atomic Orbitals	Molecular Orbitals
1. They belong to one specific atom only.	1. They belong to all atoms in a molecule.
2. They are the internal characteristics of an atom.	2. They result when atomic orbitals of similar energies combine.
3. They have simple shapes of geometries.	3. They have complex shapes.
4. Atomic Orbitals are named as s, p, d, f, etc.	4. The M.O.'s are named as: σ, π, δ, etc.
5. The stabilies of these orbitals are less than bonding & more than anti bonding orbitals.	5. The stabilies of these orbitals are either more (or) less than the Atomic Orbitals
6. Atomic Orbital is monocentric.	6. It is Polycentric.