BHARATI VIDYAPEETH DEEMED UNIVERSITY, PUNE (INDIA)

SYLLABUS OF MASTER OF SCIENCE (CHEMISTRY)

Learning Outcomes based Curriculum Framework (LOCF) for

M.Sc.I (ANALYTICAL/ORGANIC/INORGANIC CHEMISTRY)

SEMESTER-I

[CBCS- 2018 Course]

TO BE IMPLEMENTED FROM JUNE 2018

M.Sc.I (ANALYTICAL/ORGANIC/INORGANIC CHEMISTRY) SEMESTER-I (CBCS-2018 COURSE)

PGCH-101: PHYSICAL CHEMISTRY - I

Total Credits: 04

Total Lectures: 60Hrs

Course Learning Outcomes:

At the end of course student will be able to –

- CO 1: Learn second law of thermodynamics and the entropy, Free energy and chemical equilibrium, Maxwell's relation and interrelation of various thermodynamic properties
- CO 2: Discuss techniques for determination of shapes and size of macromolecules, molar mass and viscosity measurements, Adsorption of gases
- CO 3: Measurement of dipole moment and its Applications
- CO 4: Know the Collision Theory, Thermodynamic aspects, Reactive, collisions, Potential energy surfaces.
- CO 5 : Understand photochemistry, Photochemical equilibrium, Photosensitization, Flash photolysis, Photo chemistry in life processes
- CO 6: Find out Phases, components and degrees of freedom; Phase rule, Two component system , Three component system

Course Content:

1) Chemical Thermodynamics

Second law of thermodynamics and the entropy, concept as state function, change of entropy with temperature and pressure, Entropy at absolute zero, Entropy changes in spontaneous processes, Frees energy and spontaneity, Free energy and chemical equilibrium, Gibbs – Helmholts's equation. Dependence of free energy on temperature, Maxwell's relation and interrelation of various thermodynamic properties, Free energy, enthalpy and entropy of mixing in ideal and non – ideal solutions. Partial molal quantities and their experimental determinations.

2) A) Structure and Properties of Macromolecules.

Techniques for determination of shapes and size of macromolecules, use of osmotic pressure to determine the molar mass of macromolecules, Distinction between Number Average and mass average molecular weights, Ultracentrifuge and determination of shape and molar mass of macromolecules from the rate of sedimentation, use of viscosity measurements and light scattering to molar mass and shapes of macromolecules.

B) Adsorption

Adsorption of gases: Physical adsorption and chemisorption, enthalpy of adsorption, adsorption isotherms; determination of surface area; Adsorption of liquid.

3) **Dipole Moment**

Dipole moment or electrical moment, Polarization of molecules in electric field, Polarization of polar molecules in electric field, Measurement of dipole moment, Determination of molecular radius by polarization, Applications of dipole moment (a) Determination of molecular structure (b) Calculation of percentage of ionic character in the bond (c) Calculation of bond angle (d) Determination of symmetry of molecules, Bond length, Bond energy.

4) Molecular reaction Dynamics

Collision Theory, Diffusion Controlled Reactions. The reaction coordinate and transition state, Eyring equation, Thermodynamic aspects, Reactive, collisions, Potential energy surfaces.

5)Photochemistry

Introduction, Absorption of light, Types of chemical reactions, laws of photo chemistry, Consequences of light absorption: primary and secondary processes, Electronic transitions in molecules, Potential energy curves for primary photo chemical processes, Excited states, Quantum yield, Luminescence of cold light, Photoluminescence, Chemiluminescence, Photochemical equilibrium, Photosensitization, Flash photolysis, Photo chemistry in life processes, Photo conductivity, Photo polymerization, Hot atom reactions, Mechanism of photo chemical reactions.

6) Phase Rule

Phases, components and degrees of freedom; Phase rule, Two component system vapour diagrams, temperature – composition diagrams, liquid – liquid phase diagrams, liquid – solid phase diagrams, ultrapurity and controlled impurity; Three component system : trianquilar phase diagrams, partially miscible liquids, the role of added salts. (freezing mixtures, such as NaCl – water-ice, CaCl₂–water-ice)

Reference Books:

- 1) Physical Chemistry, G.M.Barrow, Fifth Edition 1994, Tata McGraw-Hill.
- 2) Physical Chemistry, P.W.Atkins, Fifth edition 1994, ELBS.
- Principles of Physical Chemistry, Maron and Prutton, Fourth edition, Macmillan Company.
- An Introduction to Electrochemistry, S. Glasstone, Affiliated East-West Press Pvt.Ltd.
- 5) Physical chemistry. R.A. Alberty, R.S.Silby, Johncoilet 1995.
- 6) Advanced Physical Chemistry, D. N. Bajpai, A. S. Chand Co. Ltd.

Note:- Weightage to the problems 25% weightage should be given to the numerical problems in final question paper setting.

PGCH-102: INORGANIC CHEMISTRY - I

Total Credits: 04

Total Lectures: 60Hrs

Course Learning Outcomes:

At the end of course student will be able to -

- CO 1: To understand structure of atom, The wave equation, particle in a box
- CO 2: Learn types of bonds, Lattice energy and size effects. Valence Band Theory, Symmetry and overlap, Hybridization
- CO 3: Understand types of solids, Band Theory, Intrinsic & photoexcited semiconductors, Impurity & defect semiconductors
- CO 4 : Applications of VSEPR theory, molecular orbitals & molecular structure and solved numericals to clear the terms.
- CO 5: Study of Inorganic Chains, Rings, Cages and Clusters
- CO 6 : Make aware of chemistry of Halogens & Noble gases

Course Content:

1. **The structure of atom:**

The wave equation, particle in a box, The Hydrogen atom: Derivation of solutions of $\theta \& \phi$ parts, solution of R part, Angular wave functions, symmetry of orbitals, the polyelectronic atom.

2. Bonding Models:

Ionic bond, Lattic energy, size effects, The covalent bond – preliminary approach, Valence Band Theory, Symmetry and overlap, Hybridization, Delocalization, Experimental measurement of charge distribution in Molecules

3. **The solid state:**

Structures of complex ionic compounds, Imperfections in crystals, conductivity in ionic solids, solids held together by covalent bonding: Types of solids, Band Theory, Intrinsic & photoexcited semiconductors, Impurity & defect semiconductors.

4. **The covalent bond: Structure & Reactivity:**

Structure of molecules, VSEPR theory, structures of molecules containing lone pairs of electrons, VSEPR rules, molecular orbitals & molecular structure, Hybridization, Bond lengths, Bond multiplicity, Experimental determination of molecular structure.

For topics 1-4, related problems should be solved in the class.

5. Inorganic Chains, Rings, Cages and Clusters:

Chains, catenation, Heterocatenation, Isopoly anions, Heteropoly anions, Rings, Borazines, Phosphazenes, Heterocyclic inorganic ring systems, Cages, Boron cage compounds, Boranes, carboranes, Metal clusters, binuclear clusters, trinuclear clusters, octahedral clusters, synthesis of metal clusters.

6. Chemistry of Halogens & Noble gases :

Introduction, Chemistry of Noble gases, bonding in noble gas halides, bond strengths in noble gas compounds

Chemistry of halogens, Interhalogen compounds, oxyacids of heavier halogens, Halogen oxides & oxyfluorides, pseudohalogens.

References

- 1. Theoretical Inorganic chemistry : M.C. Day and J. Selbin. Reinhardt EWAP (1987).
- 2. Structural Inorganic Chemistry, A.F. Wells, 5th edition (1984).
- Inorganic Chemistry Principles of structure and Reactivity: James E.Huheey, Harper and Row publisher Inc. New York, Third edition (1983).
- 4. Electronic processes in materials : L.V.Azoroff and J.J.Brophy, McGraw Hill publication.
- 5. Advanced Inorganic chemistry: F.A. Cotton, R.G.Willkinson (Wiely Eastern).
- 6. Inorganic chemistry: A.G.Sharpe, ELBS edition (1984).
- 7. Concise Inorganic chemistry: J.D.Lee, 5th edition, ELBC (1986).

PGCH-103: ORGANIC CHEMISTRY - I

Total Credits: 04

Total Lectures: 60Hrs

Course Learning Outcomes:

At the end of course student will be able to –

- CO 1: Understand SN¹, SN², SNi, SN1', SN2' &SNi' with respect to mechanism and stereochemistry
- CO 2: Learn concept of Aromaticity, Arenium ion mechanism, orientation and reactivity inaromatic electrophilic substitutions.
- CO 3: Carry out SNAr and Aryne mechanism aromatic nucleophilic substitution
- CO 4 : Mechanistic and stereochemical aspects of addition reactions of C-C multiple bonds including allenes, Ionic and free radical additions
- CO 5: Make students to understand E1, E2 & E1cB mechanisms and their orientation
- CO 6: Concept of chirality: Recognition of symmetry elements. enantiomers, diasteromers, racemic modification and their resolution, R/S nomenclature, geometrical isomerism, E & Z nomenclature,
- CO 7: Learn mechanism Rearrangements like Beckmann, Hoffmann, Schmidtetc
- CO 8: Non-Benzenoid Aromatics study

Course Content:

(1) Aliphatic Nucleophilic substitutions.

SN1, SN2, SNi, SN1', SN2' & SNi' with respect to mechanism and stereochemistry. Nucleophilic substitutions at an allylic, aliphatic and vinylic carbons. Reactivity effect of substrate structure, effect of attacking nucleophiles, leaving groups and reaction medium. Ambidient nucleophiles. Neighbouring group participation by σ , π and aromatic ring systems.

(2) Aromatic Electrophilic Substitutions.

Introduction, concept of Aromaticity, Arenium ion mechanism, orientation and reactivity in Nitration, Sulphonation, Halogenation, Friedel – Craft reactions in aromatic systems. Energy profile diagrams. The orthol / para ratio, ipso attack orientation inringsystems, Diazo-Coupling, Jakobsen, Haworth, Henkel and halogen dance reaction.

(3) Aromatic Nucleophilic Substitution.

Introduction, specificity of the reactions, SNAr, Aromatic SN1 and Aryne mechanism. Effect of substrate structure, leaving group, attacking group, base & solvent.

(4) **Addition Reaction**

Mechanistic and stereochemical aspects of addition reactions of C-C multiple bonds including allenes, Ionic and free radical additions of halogens, halogen halides & hydration. Electrophilic addition involving Metal ions, Reg io and chemo selectivity, orientation and reactivity, Conjugate addition.

(5) **Elimination Reaction**

The E1, E2 & E1cB mechanisms. Orientation in elimination reactions. Reactivity, effect of substrate structures, attacking base, leaving group, nature of medium and pyrolytic elimination reactions.

(6) **Stereochemistry**.

Concept of chirality: Recognition of symmetry elements and chiral structures. prochiral relationship. enantiomers. diasteromers. racemic modification and their resolution. R/S nomenclature, geometrical isomerism, E & Z nomenclature, conformational analysis of mono and disubstituted cyclohexanes.

(7) **Rearrangements**.

Beckmann, Hoffmann, Schmidt, Curtius, Lossen, Claisen, Fries Benzilic acid, Favorskii and wolf rearrangement.

(8) Non-Benzenoid Aromatics.

Huckel's rule and concept of aromaticity, annulenes, heteroannulenes and fullerene (C_{60}) .

Reference books.

- 1) Advanced organic chemistry by Jerry March, 4th edition, Mc Graw Hill, 1988.
- Advanced organic chemistry (Part-A) by F.A.Carey and R.J. Sundberg, 3rd edition, plenum press, New York and London, 1990.
- Modern synthetic reactions by H.O. House, 2nd edition, Benjamin / Cummings Publishing Company, 1976.
- Stereochemistry of Carbon Compounds by E.L.Eliel, 9th Reprints, Tata McGraw Hill, 1985.
- Stereochemistry, Conformations and Mechanism by P.S.Kalsi, Wiley Eastern Ltd., 2nd edition, 1993.
- Organic Reactions & their mechanism by P.S.Kalsi, 2nd edition, New Age International, 1998.