

## COURSE STRUCTURE OF THE PROGRAMME

### Semester I

Exam: 3 hours (Internal 25%, External 75%) Total Credits 12

| Sl. No | Code No. | Name of Course                 | Hours/Week | Credits |
|--------|----------|--------------------------------|------------|---------|
| 1      | PC1 C01  | INORGANIC CHEMISTRY I          | 4          | 4       |
| 2      | PC1 C02  | ORGANIC CHEMISTRY I            | 4          | 4       |
| 3      | PC1 C03  | THEORETICAL CHEMISTRY I        | 4          | 4       |
| 4      | PC1 P01  | INORGANIC CHEMISTRY PRACTICALS | 4          | -       |
| 5      | PC1 P02  | ORGANIC CHEMISTRY PRACTICALS   | 4          | -       |
| 6      | PC1 P03  | PHYSICAL CHEMISTRY PRACTICALS  | 5          | -       |
| TOTAL  |          |                                | 25         | 12      |

-

### Semester II

Exam: 3 hours (Internal 25%, External 75%) Total Credits 12

| Sl. No | Code No. | Name of Course                 | Hours/Week | Credits |
|--------|----------|--------------------------------|------------|---------|
| 1      | PC2 C04  | ORGANIC CHEMISTRY II           | 4          | 4       |
| 2      | PC2 C05  | PHYSICAL CHEMISTRY I           | 4          | 4       |
| 3      | PC2 C06  | THEORETICAL CHEMISTRY II       | 4          | 4       |
| 4      | PC1 P01  | INORGANIC CHEMISTRY PRACTICALS | 4          | 4       |
| 5      | PC1 P02  | ORGANIC CHEMISTRY PRACTICALS   | 4          | 4       |
| 6      | PC1 P03  | PHYSICAL CHEMISTRY PRACTICALS  | 5          | 4       |
| TOTAL  |          |                                | 25         | 24      |

### Semester III

Exam: 3 hours (Internal 25%, External 75%) Total Credits 16

| Sl. No                    | Code No. | Name of Course                   | Hours/Week | Credits |
|---------------------------|----------|----------------------------------|------------|---------|
| 1                         | PC3 C07  | INORGANIC CHEMISTRY II           | 4          | 4       |
| 2                         | PC3 C08  | PHYSICAL CHEMISTRY II            | 4          | 4       |
| 3                         | PC3 C09  | POLYMER CHEMISTRY                | 4          | 4       |
| 4                         | PC3E01   | POLYMER MATERIALS                | 4          | 4       |
| 5                         | PC3 P04  | POLYMER CHEMISTRY PRACTICALS I 3 | 3          | -       |
| 6                         | PC3 P05  | PHYSICAL CHEMISTRY PRACTICALS    | 3          | -       |
| PROJECT/DISSERTATION WORK |          |                                  | 3          | -       |

|       |    |    |
|-------|----|----|
| TOTAL | 25 | 24 |
|-------|----|----|

#### Semester IV

Exam: 3 hours (Internal 25%, External 75%) Total Credits 28

Sl.

| Sl. No                                  | Code No. | Name of Course  | Hours/Week | Credits   |
|---|----------|---|------------|-----------|
| 1                                       | PC4 C10  | PHYSICAL CHEMISTRY OF POLYMERS  | 4          | 4         |
| 2                                       | PC4 C11  | POLYMER TECHNOLOGY  | 4          | 4         |
| 3                                       | PC4 C12  | TESTING AND CHARACTERIZATION OF POLYMERS                                | 4          | 4         |
| 4                                       | PC4E02   | PLASTIC AND FIBER TECHNOLOGY<br><b>OR</b><br>ii) POLYMER NANOTECHNOLOGY | 4          | 4         |
| 5                                       | PC4 P04  | POLYMER CHEMISTRY PRACTICALS I  | 3          | 2         |
| 6                                       | PC4 P05  | POLYMER CHEMISTRY PRACTICALS II   | 3          | 2         |
| PROJECT/DISSERTATION WORK               |          |   | 3          | 5         |
| VIVA VOCE                               |          |   |            | 3         |
|   |          |   |            |           |
| TOTAL                                   |          |   | 25         | 28        |
| <b>TOTAL CREDITS FOR THE PROGRAMME:</b> |          |   |            | <b>80</b> |

**UNIVERSITY OF CALICUT**  
**M. Sc. POLYMER CHEMISTRY- SEMESTER I**  
**PC1 C 01 INORGANIC CHEMISTRY- I Credits: 4**

**MODULE I (7 h)**

Acid base theories - strength of acids and bases, solvent leveling effect, hard and soft acids and bases, super acids. Chemistry of non-aqueous solvents- liquid  $\text{NH}_3$ ,  $\text{SO}_2$ ,  $\text{H}_2\text{SO}_4$  and  $\text{HF}$ . Heterogeneous acid- base reactions- surface acidity, solid- and molten acids in industrial processes.

**MODULE II (8 h)**

Boranes-Classification, Synthesis, structure, reactions and bonding in boron hydrides-carboranes, metalloboranes and borazines, styx number, Wade- Mingos Rule. Synthesis, structure and applications of silicones. Phosphorus- nitrogen, phosphorus- sulphur and sulphur-nitrogen ring and chain compounds- synthesis, structure, bonding and applications.

**References (MODULE I and II)**

1. D. F. Shriver, P. W. Atkins, C. H. Langford, *Inorganic Chemistry*, ELBS, 1990.
2. J. E. Huheey, E. A. Keiter, R. L. Keiter, *Inorganic chemistry, Principles, Structure and Reactivity*, Pearson Education, 1990.
3. F. A. Cotton, G. Wilkinson, *Advanced Inorganic Chemistry*, 5th Edn., John Wiley and sons, 1988.

**MODULE III (20 h)**

Crystalline solids, crystal systems, Bravais lattices, crystal symmetry, symmetry elements, transitional and rotational transition symmetry, point groups, space groups, indices, Bragg's law, X- ray diffraction. Close packing, factors affecting crystal structure, radius ratio, coordination number, lattice energy, Born- Haber cycle, structure of  $\text{AX}$ ,  $\text{AX}_2$ ,  $\text{AO}_2$ ,  $\text{AO}_3$ ,  $\text{A}_2\text{O}_3$ ,  $\text{ABO}_3$ ,  $\text{AB}_2\text{O}_4$  type crystal defects, non- stoichiometry, sharing of polyhedra, structure of silicates, aluminosilicates, molecular sieves, polyoxyanions.

Electronic properties of solids, band theory, k- space, Brillouin zones, band structure. Fermi level, Fermi energy, density of states, metals, insulators, semiconductors, types and structure of semiconductors, super conductors. Alloys, classification, intermetallic compounds, Hume Rothery rules.

Solid state reactions, solid-solid, solid-gas and solid-liquid reactions, kinetics, thermal analysis, borides, carbides, silicides, preparation and properties, preparative methods in solid state chemistry.

**References**

1. A. R. West, *Solid State Chemistry and its Applications*, John- Wiley, Chichester, 1984.
2. F. D. Bloss, *Crystallography and Crystal Chemistry*, Holt Reinhart, Winston, New York, 1971.
3. A. F. Wells, *Structural Inorganic Chemistry*, Clarendon Press, Oxford, 1954.
4. A. K. Galway, *Chemistry of Solids*, Chapman- Hall, London, 1967.
5. M. F. C. Ladd, *Structure and Bonding in Solid State Chemistry*, Ellis Harwood, Chichester, 1979.
6. P. A. Cox, *The Electronic Structure and Chemistry of Solids*, Oxford University Press.
7. L. V. Azaroff, *Introduction to Solids*. McGraw Hill, 1960.

#### **MODULE IV Nuclear Chemistry (10 h)**

Radioactive decay and equilibrium- nuclear reactions- Q value, types of reactions, chemical effects of nuclear transformation,  $\alpha$ - recoil- effects of radiation on materials fission and fusion, fusion products and fusion yields- Radioactive techniques, tracer techniques- neutron activation analysis- Principle and working of GM counter, scintillation counters, ionization and proportional counter.

#### **References**

1. J. B. Rajam, *Atomic Physics*, S. Chand and Co. Pvt. Ltd., 1974.
2. J. W. T. Spinks, R. J. Woods, *An Introduction to Radiation Chemistry*, John Wiley and Sons, 1964.
3. H. J. Anikar, *Essentials of Nuclear Chemistry*, 4th Edn., New Age International, 1995.
4. S. Glasston, *Source Book on Atomic Energy*, 3rd Edn., East- West Press Pvt. Ltd., 1967.
5. Friedlander, J. W. Kennedy, *Introduction to Radiochemistry*, John Wiley and Sons, 1981.
6. Friedlander, J. W. Kennedy, J. M. Miller, *Nuclear and Radiochemistry*, 3rd Edn., John Wiley and Sons, 1981.

#### **MODULE V (6 h)**

Errors and treatment of analytical data, standard deviation, least square analysis, statistical treatment of data sets, students tests, confidence limit,  $Q$  test.

Theory of acid- base-, redox-, adsorption- and complexometric indicators, titrations in non-aqueous solvents.

#### **References**

1. G. H. Jeffery, J. Bassett, J. Mendham, R. C. Denny, *Vogel's Text book of Quantitative Chemical Analysis*, 5th Edn., ELBS, 1989.
2. Skoog, West, Holler, *Fundamentals of Analytical Chemistry*, 8th Edn., Thomson and Brooks, 2004.

#### **MODULE VI (11 h)**

Coordination chemistry formation and stability of complexes, Stepwise and overall formation constants and the relationship between them. Determination of binary formation constants. Chelate and macrocyclic effect. The crystal field and ligand field theories, orbital splitting in octahedral, tetrahedral and square planar fields, spectrochemical- and nephelauxetic series, Racah parameters. Jahn-Teller effect. M.O. theory- composition of ligand group orbitals. M.O. diagrams of complexes with and without p- bonding.

Spectroscopic term symbols of molecules

#### **References ( MODULE VI and VII)**

1. D. F. Shriver, P. W. Atkins, C.H. Langford, *Inorganic Chemistry*, ELBS, 1990.
2. J. E. Huheey, E. A. Keiter, R. L. Keiter, *Inorganic Chemistry, Principles, Structure and Reactivity*, Pearson Education, 1990.
3. F. A. Cotton, G. Wilkinson, *Advanced Inorganic Chemistry*, 5th Edn., John Wiley and Sons, 1988.

**MODULE VII (10 h)**

Chemistry of transition and inner transition elements -Heteropoly and isopoly anions of W, Mo, V. Standard reduction potentials and their diagrammatic representations Ellingham diagram. Latimer and Frost diagrams. Pourbaix diagram.

Lanthanides and actinides- stable oxidation states, the lanthanide and actinide contraction, the f orbitals, lanthanide chelates, separation of lanthanides and actinides, transactinide elements.

**References ( MODULE VI and VII)**

1. D. F. Shriver, P. W. Atkins, C.H. Langford, *Inorganic Chemistry*, ELBS, 1990.
2. J. E. Huheey, E. A. Keiter, R. L. Keiter, *Inorganic Chemistry, Principles, Structure and Reactivity*, Pearson Education, 1990.
3. F. A. Cotton, G. Wilkinson, *Advanced Inorganic Chemistry*, 5th Edn., John Wiley and Sons, 1988.

**MODULE WISE WEIGHTAGE FOR QUESTIONS**

| MODULE | WEIGHTAGE |
|--------|-----------|
| I      | 5         |
| II     | 5         |
| III    | 14        |
| IV     | 7         |
| V      | 5         |
| VI     | 7         |
| VII    | 7         |

## **PC1 C02 ORGANIC CHEMISTRY I Credits: 4**

### **MODULE I (10 h)**

Delocalised chemical bonding, Electron Delocalization, Resonance and Aromaticity: Qualitative application of Huckel MO theory and perturbation theory to systems containing delocalized electrons. Delocalized electrons and Resonance, Resonance hybrid and resonance energy. Criteria for Aromaticity and Antiaromaticity, MO description of Aromaticity and Antiaromaticity. Homoaromaticity, Mobius twist and Aromaticity. Aromaticity of Annulenes and heteroannulenes, Fullerenes, and fused ring systems. Stability of benzylic cations and radicals, Effect of delocalized electrons on pK<sub>a</sub>.

#### *Hydrogen Bonding:*

Inter- and intramolecular hydrogen bonding. Range of the energy of hydrogen bonding. Volatility, acidity, basicity and stability of hydrates of carbonyl compounds. Stabilization of hydrates of glyoxal and chloral, and ninhydrin. Comparison of boiling points of ethanol and dimethyl ether (two isomeric compounds). High volatility of *o*-nitrophenol and salicylaldehyde compared to their *meta*- and *para*- isomers. High acid strength of maleic acid compared to fumaric acid.

### **MODULE II (10 h)**

#### *Basic Concepts in the Study of Organic Reaction Mechanisms*

Application of Experimental criteria to mechanistic studies, Thermodynamic and kinetic data, Curtius- Hammet principles, Kinetic versus thermodynamic control. Acidity constant, Hammet acidity function. Reactive intermediates and their characterization. Isotope effect (labeling experiments), stereochemical correlations. Structure and reactivity, Transition state theory, Potential energy vs Reaction coordinate curve, Substituent effects (inductive, mesomeric, inductomeric, electomeric and field effects) on reactivity. Qualitative study of substitution effects changing with mechanism in S<sub>N</sub>1 – S<sub>N</sub>2 reactions. Semi quantitative study of substituent effects on the acidity of carboxylic acids. Quantitative correlation of substituent effects on reactivity. Linear free energy relationships. Hammet and Taft equation for polar effects and Taft's steric substituent constant for steric effect.

#### **References (MODULE I and II)**

1. J. March, *Advanced Organic Chemistry*, 4th Edn., John Wiley and sons, 1992.
2. T. H. Lowry, K. S. Richardson, *Mechanism and Theory in Organic Chemistry*, HarperCollins, 1987.
3. F. A. Carey, R. J. Sundberg, *Advanced Organic Chemistry (Parts A & B)*, 3rd Edn., Plenum Press, 1990.
4. R. A. Y. Jones, *Physical and Mechanistic Organic Chemistry*, Cambridge University Press, 1979.

### **MODULE III Isomerism (10 h)**

Dissymmetry, asymmetry and chirality- simple and alternating axis of symmetry- Conditions for optical activity, Isotopic asymmetric variation and specific rotation of the same compound in sign

and magnitude under different conditions. Relative and absolute configurations. Sequence rule—R and S notations in cyclic and acyclic compounds.

Optical isomerism of compounds containing one or more asymmetric carbon atoms, Enantiotopic, Homotopic, Diastereotopic hydrogen atoms, Prochiral centre. Optical isomerism in Biphenyls: Structure of biphenyls in solid, liquid and vapour states. Structure of substituted biphenyls. Number of substituent's and their size in relation to the stability of optical isomers. R and S notation. Atropisomers. Restricted rotation in biphenyls – Molecular overcrowding. Chirality due to folding of helical structures. Conditions for optical activity in allenes and spiro compounds- R and S notation. Optical isomerism of nitrogen and sulphur compounds- naming- stereochemistry. Conditions for optical activity, R and S notation.

Geometrical isomerism –

E and Z notation of compounds with one and more double bonds in acyclic systems. Methods of determination of the configuration of geometrical isomers in acyclic and cyclic systems, interconversion of geometrical isomers. Stereochemistry of aldoximes and ketoximes – naming – isomerism – methods of determining configurations of aldoximes and ketoximes.

### References

1. J. March, *Advanced Organic Chemistry*, 4th Edn., John Wiley and Sons, 1992.
2. Nasipuri, *Stereochemistry of Organic Compounds*, 2nd Edn., New Age International.
3. Kalsi, *Stereochemistry of Organic Compounds*, Wiley Eastern.

### Suggested Reading

E. Eliel, S. H. Wilen, *Stereochemistry of Organic Compounds*, John Wiley, 1994.

### MODULE IV Conformational Analysis (16 h)

Conformation and configuration. Internal factors affecting the conformation dipolar interaction, bond opposition strain, bond angle strain, intra molecular hydrogen bonding.

Sawhorse and Newman projections. Eclipsed, gauche and staggered conformations. Conformations of acyclic compounds – Ethane, *n*-butane, ethylene dihalide, glycols, chlorohydrins, *meso* and *dl*-tartaric acids, acetaldehyde and acetone.

Conformation of cyclohexane, conformations of mono- and di- substituted cyclohexanes, conformation of decalins, and 2-halocyclohexanones. Anchoring group. Effect of conformation on reactivity – Debromination of *dl* and *meso*-2,3-dibromobutane with KI, dehydrogenation of stilbene dihalides (*dl* and *meso*) and erythro- and threo-1-bromo-1,2-diphenylpropane. Effect of conformation on the course and rate of reactions – SN1 and SN2 reactions of axial and equatorial substituents. E1 and E2 eliminations of

(i) 4-*t*-Butylcyclohexyl tosylates (*cis* and *trans*)

(ii) 2-Phenylcyclohexanols

(iii) Menthyl and *neomenthyl* chlorides, and benzene hexachlorides.

Esterification of axial and equatorial alcohols and acids- their hydrolysis. ORD and CD. Plane and single CE curves- uses. Axial haloketone rule and its application. Octant rule- Determination of conformation and configuration of 3-Methylcyclohexanone- ORD curves of *cis*- and *trans*-decalones.

### References

1. Nasipuri, *Stereochemistry of Organic Compounds*, 2nd Edn., New Age International.
2. Eliel, Allinger, Anggal, Morrison, *Conformational analysis*, Wiley International.

3. I. L. Finar, *Organic Chemistry, Vol. II*, 5th Edn., ELBS, 1975.

### **MODULE V Reactions of Carbon-Heteromultiple Bonds (6 h)**

Addition to carbon-oxygen multiple bond: Addition of water, alcohols, amines and hydrazine. Aldol, Claisen, Dieckmann, and Stobbe condensation. Darzen, Knoevenagel, Wittig, Mannich and Prins reactions. MPV reduction and Oppenau oxidation. Cram's rule. Hydrolysis, alcoholysis and reduction of nitriles. Ritter reaction and Thorpe condensation. Clemmenson and Wolf-Kishner reduction.

#### **References**

1. J. March, *Advanced Organic Chemistry*, 4th Edn., John Wiley and sons, 1992.
2. Morrison, Boyd, *Organic Chemistry*, Prentice Hall.
3. F. A. Carey, R. J. Sundberg, *Advanced Organic Chemistry (Parts A & B)*, 3rd Edn., Plenum Press, 1990.

### **MODULE VI (14 h)**

#### **i) Electrophilic and Nucleophilic substitution in aromatic systems. (7 h)**

Friedel-Crafts alkylation and acylation. Orientation in monosubstituted benzene. *Ortho-para* ratio with reference to electronegativity and steric factors. Nucleophilic aromatic substitution, Aromatic diazonium ions as synthetic intermediates. Nucleophilic substitution as illustrated by the hydrolysis of 2,4-dinitro-chlorobenzene. Amination of pyridine by sodamide (Chichibabin reaction). Aryne mechanism. Examples, Detection of benzyne intermediate, orientation of addition. Structure of benzyne.

#### **ii) Nucleophilic Substitution at Saturated Carbon and Elimination Reactions (7 h)**

The four types of nucleophilic substitution reactions based on charges on the nucleophile and leaving group. Nucleophilicity and size of nucleophile. Effect of changing the basic nature of the leaving group. Effect of solvent polarity - solvent effects on nucleophilic substitution of different charge types due to Ingold Y-value and Dimroth parameter. Stereochemistry of SN1 and SN2 reactions. Reactions of epoxides and quaternary ammonium compounds. Neighbouring group participation- participation of carboxylate ion, halogen, hydroxyl group, acetoxy group, phenyl group and p bond. Elimination at Bridgehead carbon - Bredt's rule. *Cis* elimination - pyrolysis of esters and Chugaev reaction. E1cB mechanism

#### **References**

1. J. B. Hendrickson, D. J. Cram, G. S. Hammond, *Organic Chemistry*, McGraw Hill International Book Company, 1981.
2. Morrison, Boyd, *Organic Chemistry*, Prentice Hall.
3. J. March, *Advanced Organic Chemistry*, 4th Edn., John Wiley and Sons, 1992.
4. J. B. Hendrickson, D. J. Cram, G. S. Hammond, *Organic Chemistry*, McGraw Hill International Book Company, 1981.
5. Morrison, Boyd, *Organic Chemistry*, Prentice Hall.
6. J. March, *Advanced Organic Chemistry*, 4th Edn., John Wiley and Sons, 1992.
7. F. A. Carey, R. J. Sundberg, *Advanced Organic Chemistry (Parts A & B)*, 3rd Edn., Plenum Press, 1990.

### **MODULE VII Photochemical and Electrochemical Synthesis. (6 h)**

Basic concepts of electroorganic reactions. Electrochemical oxidation and reduction reactions. Cathodic reduction of organic functional groups like halo, nitro etc. Electrodimerisation and electropolymerisation reactions. Electrochemical sensors. Electrooxidations. Industrial applications of organic photochemistry.

#### **References**



1. A. J. Fry, *Synthetic Organic Electrochemistry*, Harper and Row Publishers, New York.
2. R. O. Kan, *Organic Photochemistry*, Mc Graw Hill.
3. D. R. Julian, *Industrial Aspects of Heterocyclic Photochemistry*, (O. Buchardt Ed.), Wiley Interscience, New York.

#### MODULE WISE WEIGHTAGE FOR QUESTIONS

| MODULE | WEIGHTAGE |
|--------|-----------|
| I      | 7         |
| II     | 7         |
| III    | 7         |
| IV     | 11        |
| V      | 4         |
| VI     | 10        |
| VII    | 4         |

## **PC1 C 03 THEORETICAL CHEMISTRY I Credits: 4**

### **MODULE I (10 h)**

#### *i) Mathematical Concepts (5 h)*

Co-ordinate systems: Cartesian, cylindrical polar and spherical polar coordinates and their relationships. Complex numbers: definition, complex conjugate, absolute value of a complex number, complex functions. Operator algebra: linear and non linear operators, Hermitian operators,  $\nabla$  and  $\nabla^2$  operators. Eigen function and Eigen values of an operator, Eigen value equation, Eigen functions of commuting operators. Well behaved functions, Normalized and Orthogonal functions.

#### *ii) Quantum Mechanics - A Historical Sketch (5 h)*

Blackbody radiation and Planck's quantum postulate. Einstein's quantum theory of radiation, Milliken's verification of Einstein's photoelectric equation, Wave-particle duality of radiation. Compton effect. Louis de Broglie's matter waves, Electron diffraction. Heisenberg's matrix mechanics (mention only), Uncertainty principle. Schrodinger's wave mechanics, Deduction of Schrodinger equation from classical wave equation.

### **MODULE II (8 h)**

#### *i) Postulates of Quantum Mechanics (4 h)*

Detailed discussion of postulates: State function postulate. Operator postulate. Eigen value postulate. Expectation value postulate. Postulate of time dependent Schrodinger equation of motion, Conservative system and time-independent Schrodinger equation.

#### *ii) Quantum Mechanics of Translational Motion (4 h)*

Particle in a one-dimensional box, important features of the problem. Symmetry of the wave functions. Particle in a three-dimensional box, Separation of variables, Degeneracy, Symmetry breaking. Introduction to Tunneling.

### **MODULE III (10 h)**

#### *i) Quantum Mechanics of Vibrational Motion (5 h)*

Harmonic oscillator (complete treatment): Method of power series, Hermite equation and Hermite polynomials, Recursion formula, Rodrigue's formula, Wave functions and energies. Important features of the problem. Harmonic oscillator and molecular vibrations. Three-dimensional harmonic oscillator.

#### *ii) Quantum Mechanics of Rotational Motion (5 h)*

Rigid rotator (complete treatment): The wave equation in spherical polar coordinates. Planar rigid rotator (or Particle on a ring), The  $\Phi$ -equation, Solution of the  $\Phi$  equation, Handling of Imaginary wave functions, Wave functions in the real form, Polar diagrams.

Non-planar rigid rotator (or particle on a sphere), Separation of variables, The  $\Phi$  equation and the  $\Theta$ -equation and their solutions, Legendre and Associated Legendre equations, Legendre and Associated Legendre polynomials, Spherical harmonics (Imaginary and real forms). Polar diagrams of spherical harmonics. Spherical harmonics as eigen functions of angular momentum

operators  $L^2$  and  $L_z$ , Quantisation of angular momentum, Angular momentum quantum numbers, Ladder operator method for angular momentum, Space quantization.

9

#### **MODULE IV (11 h)**

##### *Quantum Mechanics of Hydrogen-Like Atoms*

Potential energy of hydrogen-like systems. The wave equation in spherical polar coordinates, Separation of variables. The  $R$ ,  $\Theta$  and  $\Phi$  equations and their solutions, Laguerre and Associated Laguerre polynomials, Wave functions and energies of hydrogen-like atoms, Orbitals. Radial functions and Radial distribution functions and their plots, Angular functions (Spherical harmonics) and their plots, Orbital diagrams. Explanation of Hydrogen spectrum, Fine structure, The postulate of spin by Uhlenbeck and Goudsmith, Dirac's Relativistic Schrodinger equation for hydrogen atom and discovery of spin, Hydrogen wave functions including spin or Spin orbitals, Construction of Spin orbitals from Orbitals and Spin functions.

#### **MODULE V (12 h)**

##### *i) Quantum Mechanics of Many- Electron Atoms and Approximation Methods (6 h)*

Many-body problem, Approximation methods. Independent particle model, Distribution of electrons in many electron atoms, Stoner's rule. Variation method, Variation theorem with proof, Illustration of variation theorem using a trial function [e.g.,  $x(a-x)$ ] for particle in a 1D-box, Variation treatment for the ground state of Helium atom, Effective nuclear charge. Perturbation method, Time-independent perturbation method (non-degenerate case only), Illustration by application to particle in a 1D-box with slanted bottom, Perturbation treatment of the ground state of the helium atom. Hartree-Fock Self-Consistent Field (HF-SCF) method. Slater's treatment of complex atoms, Slater Orbitals, Slater's rules for calculating Slater orbitals.

##### *ii) Electron Spin in Many-Electron Atoms (3 h)*

Construction of wave functions including spin for many electron atoms, Symmetric and antisymmetric wave functions, Pauli's antisymmetry principle, Slater determinants, Pauli's exclusion principle.

##### *iii) Vector Model of Atoms and Spectroscopic Terms (3 H)*

Coupling of angular momenta, LS and JJ- couplings, LS coupling and Spectroscopic term symbols for atoms. Electronic spectrum of hydrogen atom - the fine structure of  $H\alpha$  line of the Balmer series.

#### **MODULE VI Chemical Bonding I (11 h)**

##### *i) Schrodinger equation for a molecule, Born - Oppenheimer approximation. (2 h)*

##### *ii) Molecular Orbital (MO) theory (4 h)*

MO theory of  $H_2^+$ . MO theory of  $H_2$ . MO treatment of homonuclear diatomic molecules  $Li_2$ ,  $Be_2$ ,  $C_2$ ,  $N_2$ ,  $O_2$ ,  $F_2$  and heteronuclear diatomic molecules  $LiH$ ,  $CO$ ,  $NO$ ,  $HF$ . Correlation diagrams, Noncrossing rule. Spectroscopic term symbols for diatomic molecules.

##### *iii) Valence Bond (VB) theory (5 h)*

VB theory of  $H_2$ . VB theory of more complex molecules: Bonding in  $BeH_2$ ,  $H_2O$ ,  $NH_3$ , orbital overlap. Molecular geometry, Hybridization, Examples: Methane, Water, Ethylene, and Acetylene, Multiple bonds, VSEPR theory.

#### **MODULE VII Chemical Bonding II (10 h)**

##### *i) MO Theory for More Complex Molecules (6 h)*

HMO theory of linear conjugated hydrocarbons (Ethylene, Butadiene, Allylic anion), Charge on an atom, bond order, Calculation of free valence. HMO theory of aromatic hydrocarbons (benzene). Formula for the roots of the Huckel determinantal equation, Frost-Huckel circle mnemonic device for cyclic polyenes.

ii) *Intermolecular Forces* (5 h)

Intermolecular forces - ion dipole, dipole-dipole, ion-induced dipole, dipole induced dipole and dispersion interactions - mathematical expressions – donor acceptor interactions - Lennard Jones potential.

**References**

1. F. L. Pilar, *Elementary Quantum Chemistry*, McGraw-Hill, 1968.
2. P. W. Atkins, *Molecular quantum mechanics*, 2nd Edn., Oxford University Press, 1983.
3. M. W. Hanna, *Quantum mechanics in Chemistry*, 2nd Edn., W. A. Benjamin Inc., 1969.
4. I. N. Levin, *Quantum Chemistry*, 5th Edn., Pearson Education Inc., 2003.
5. D. A. McQuarrie, *Quantum Chemistry*, University Science Books, 1983.
6. J. P. Lowe, *Quantum Chemistry*, 2nd Edn., Academic Press Inc., 1993.
7. A. K. Chandra, *Introduction to Quantum Chemistry*, Tata McGraw-Hill, 1994.
8. L. Pauling, E. B. Wilson, *Introduction to Quantum Mechanics*, McGraw-Hill, 1935 (A good source book for many derivations).
9. R. L. Flurry, Jr., *Quantum Chemistry*, Prentice Hall, 1983.
10. R. K. Prasad, *Quantum Chemistry*, 2nd Edn., New Age International, 2000
11. M. S. Pathania, *Quantum Chemistry and Spectroscopy (Problems & Solutions)*, Vishal publications

| MODULE | WEIGHTAGE |
|--------|-----------|
| I      | 7         |
| II     | 6         |
| III    | 7         |
| IV     | 7         |
| V      | 8         |
| VI     | 8         |
| VII    | 7         |

**M. Sc. POLYMER CHEMISTRY- SEMESTER II**  
**PC2 C 04 ORGANIC CHEMISTRY II Credits: 4**

**MODULE I *Pericyclic Reactions* (10 h)**

Definition and types of pericyclic reactions a) cycloaddition and cycloreversion (b) electrocyclic ring closure and ring opening c) sigmatropic rearrangement. Stereochemistry of pericyclic reactions and theory of molecular orbital symmetry. Application of theory of molecular orbital symmetry by the method of correlation diagram for cycloaddition and electrocyclic reactions by both thermal and photochemical paths. Stereochemistry of pericyclic reactions- thermal and photochemical by method of transition state aromaticity. Stereochemistry of pericyclic reactions by FMO. Selection rules. Sommelet-Hauser, Cope and Claisen rearrangements.

**References**

1. T. H. Lowry, K. S. Richardson, *Mechanism and Theory in Organic Chemistry*, HarperCollins.
2. S. H. Pine, J. B. Hendrickson, D. J. Cram, G. S. Hammond, *Organic Chemistry*, McGrawHill International Book Company, 1981.
3. F. A. Carey, R. J. Sundberg, *Advanced Organic Chemistry (Parts A & B)*, 3rd Edn., Plenum Press, 1990.

**MODULE II *Chemistry of Free Radicals and Photochemistry* (12 h)**

- i) Stability of free radicals. Formation and detection of free radicals. Structure and stereochemical properties of radical intermediates characteristics and reaction mechanism involving radical intermediates. Free radical substitution and addition reactions. Rearrangement and fragmentation reactions. Carbenes and nitrenes.
- ii) Fundamental Concepts, Molecular excitation, Jablonski diagram and the singlet and triplet states. Photosensitization. Reactions involving the olefinic double bonds, reactions of carbonyl compounds and reactions of aromatic compounds. Photoreduction. Di-pi-methane rearrangement. Barton reaction and photo Fries rearrangement. Mechanism of photosynthesis, photochemistry of dyes and pigments, photochemistry of vision.

**References**

1. T. H. Lowry, K. S. Richardson, *Mechanism and Theory in Organic Chemistry*, Harper Collins.
2. J. March, *Advanced Organic Chemistry*, 4th Edn., John Wiley and sons, 1992.
3. F. A. Carey, R. J. Sundberg, *Advanced Organic Chemistry (Parts A & B)*, 3rd Edn., Plenum Press, 1990.
4. R. O. Kan, *Organic Photochemistry*, McGraw Hill.
5. O. L. Chapman, *Organic Photochemistry Vol. I & II*, Marcel Decker.
6. F. A. Carey, R. J. Sundberg, *Advanced Organic Chemistry (Parts A & B)*, 3rd Edn., Plenum Press, 1990.

12

**MODULE III *Molecular Rearrangements* (6 h)**

Rearrangement involving electron deficient carbon, nitrogen and oxygen atoms, Wagner-Meerwein, Dienone-phenol, Wolff, Hoffmann, Curtius, Lossen, Beckmann, Schmidt and Baeyer-Villiger rearrangements. Anionic rearrangements: Benzil-benzilic acid and Favorski rearrangements. Orton, Claisen and Fries rearrangements.

### References

1. P. Sykes, *A Guide Book to Mechanisms in Organic Chemistry*, Orient Longmans, 2002.
2. S. H. Pine, J. B. Hendrickson, D. J. Cram, G. S. Hammond, *Organic Chemistry*, McGraw Hill International Book Company, 1981.
3. J. March, *Advanced Organic Chemistry*, 4th Edn., John Wiley and sons, 1992.

### MODULE IV *Organic Spectroscopy* (18 h)

Application of UV, IR, NMR, and MS in the structure elucidation of organic compounds. Problem solving approach (Instrumentation not required).

*UV*: Characteristic absorption of organic compounds - Empirical rules for calculating absorption maxima of dienes and enones.

*IR*: Characteristic group absorptions of organic molecules - Alkanes, alkenes, alkynes, mononuclear aromatic hydrocarbons, alcohols, phenols, ethers, carbonyl compounds, amines, amides and nitriles.

*NMR*: The chemical shift, Local diamagnetic shielding and magnetic equivalence. Spin-spin coupling and coupling constants. Coupling of protons to other nuclei -quadrupole broadening. First and second order spectra. Homotopic, enantiotopic and diastereotopic protons. Spin decoupling and double resonance, Vicinal and germinal coupling in rigid systems. High resolution NMR. <sup>13</sup>C chemical shifts. Correlation charts. Proton coupled, off resonance decoupled and noise- decoupled spectra.

*MS*: Determination of molecular mass. Molecular formula from isotope ratio. fragmentation pattern in different classes of compounds. Modern techniques of ionization.

### References

1. R. M. Silverstein, G. C. Bassler, T. C. Morrill, *Spectroscopic Identification of Organic Compounds*, John Wiley and Sons Inc., 1991.
2. W. Kemp, *Organic Spectroscopy*, 3rd Edn., McMillan. 1991.
3. P. S. Kalsi, *Spectroscopy of Organic Compounds*, New Age International, 1998.

### MODULE V *Organic Reactions and Mechanisms* (8 h)

Robinson annulation, Birch reductions, hydroboration, Favorski reaction, Stork enamine reaction, Michael addition, Sharpless asymmetric epoxidation, Hofmann-Löffler- Freytag reaction, Shapiro reaction and Bayer- Villiger reaction.

### References

1. F. A. Carey, R. J. Sundberg, *Advanced Organic Chemistry (Parts A & B)*, 3rd Edn., Plenum Press, 1990.
2. H. O. House, *Principles of Organic Synthesis*.
3. J. March, *Advanced Organic Chemistry*, 4th Edn., John Wiley and sons, 1992.

13

### MODULE VI *Heterocyclic Compounds and Natural Product Chemistry* (8 h)

Structure, synthesis and reactions of pyrazole, imidazole and thiazole. Synthesis of uracil, thymine, cytosine, adenine, guanine, caffeine and pyrazine. Biosynthesis of alkaloids, terpenoids, steroids, carbohydrates and proteins.

### Reference

1. I. L. Finar, *Organic Chemistry Vol. II*, 5th Edn., ELBS, 1975.

**MODULE VII *Synthetic Reagents* (10 h)**

Uses of the following reagents in organic synthesis. Complex metal hydrides. Gilman's reagent, lithium diisopropyl amide (LDA), DCC, 1,3-Dithiane (reactivity umpolung), trimethylsilyl iodide, tri-n-butyl tin hydride, OsO<sub>4</sub>, DDQ, SeO<sub>2</sub>, Woodward and Prevost hydroxylation, phase transfer catalysts, crown ethers and Merrifield resin, Peterson's synthesis, Wilkinson catalyst and Baker yeast.

**References**

1. F. A. Carey, R. J. Sundberg, *Advanced Organic Chemistry (Parts A & B)*, 3rd Edn., Plenum Press, 1990.
2. H. O. House, *Principles of Organic Synthesis*.
3. J. March, *Advanced Organic Chemistry*, 4th Edn., John Wiley and sons, 1992.

**MODULE WISE WEIGHTAGE FOR QUESTIONS**

| MODULE | WEIGHTAGE |
|--------|-----------|
| I      | 7         |
| II     | 8         |
| III    | 4         |
| IV     | 13        |
| V      | 5         |
| VI     | 6         |
| VII    | 7         |

## **PC2 C 05 PHYSICAL CHEMISTRY I Credits: 4**

### **MODULE I Thermodynamics I (12 h)**

i) Review of first and second laws. Third law of thermodynamics, need for the third law, Nernst heat theorem, Apparent exceptions to third law, Applications of third law, Determination of absolute entropies, Residual entropy. Determination of relations connecting the thermodynamic partial derivatives by the method of Jacobians (discussion to be confined to closed thermodynamic systems).

#### *ii) Thermodynamics of Solutions*

Partial molar quantities, Chemical potential, Variation of Chemical Potential with temperature and Pressure, Partial molar volume and its determination, Gibbs-Duhem equation, Thermodynamics of ideal and real gases and gas mixtures. Fugacities of gases and their determinations, Activity, activity coefficient, standard states of substances (for solute and solvents). Duhem-Margules equation and its applications. Thermodynamics of ideal solutions, Deductions of the laws of Raoult, ebullioscopy, cryoscopy and osmotic pressure. Non-ideal solutions, Deviations from Raoult's law, Excess functions - excess free energy, excess entropy, excess enthalpy and excess volume.

### **MODULE II Thermodynamics II (8 h)**

#### *Thermodynamics of Irreversible Processes*

Simple examples of irreversible processes. General theory of non-equilibrium processes. Entropy production. The phenomenological relations. Onsager reciprocal relations, Application to the theory of diffusion, thermal diffusion, thermosmosis and thermomolecular pressure difference, Electrokinetic effects. The Glansdorf-Prigogine equation.

### **References (MODULE I & II)**

1. S. Glasstone, *Thermodynamics for Chemists*, East-West, 1973
2. Rajaram, Kuriokose, *Thermodynamics*, East-West, 1986
3. R. P. Rastogi, R. R. Misra, *An Introduction to Chemical Thermodynamics*, New Age International.
4. D. A. McQuarrie, J. D. Simon, *Physical Chemistry, A Molecular Approach*, University Science Books, 1997.
5. K. J. Laidler, J. H. Meiser, B. C. Sanctuary, *Physical Chemistry*, Houghton Mifflin Company, New York, 2003.
6. Prigogine, *An Introduction to Thermodynamics of Irreversible Processes*, Interscience.
7. B. G. Kyle, *Chemical and Process Thermodynamics*, 2nd Edn., Prentice Hall of India.
8. G. K. Vemulapalli, *Physical Chemistry*, Printice Hall of India.

### **MODULE III Electrochemistry – I (10 h)**

i) Debye-Huckel theory of electrolytic conduction - Derivation of Debye-Huckel- Onsager equation. Deviation from Debye-Huckel-Onsager equation and corrections. Degree of dissociation and its determination. Conductance ratio. Debye-Falkenhagen effect, Wein effect.



ii) Activity and activity coefficients of electrolytes. Ionic strength, variation of activity coefficient with concentration, Derivation of Debye-Huckel limiting law and its various forms, Qualitative and quantitative tests of the Debye- Huckel limiting law.

#### **MODULE IV *Electrochemistry – II* (10 h)**

Polarization, overvoltage and polarography. Electrolytic polarization, dissolution and deposition potentials, concentration polarization. Decomposition voltage and its determination. Over voltage - hydrogen over voltage, oxygen overvoltage, metal deposition over voltage and their determination. Theories of over voltage – Ionic diffusion as the slow process - Principles of polarography, dropping mercury electrode, the half wave potential. Electrode kinetics.

##### **References**

1. S. Glasstone, *Introduction to Electrochemistry*, East-West Press Pvt. Ltd., 1965
2. D. A. McInnes, *The Principles of Electrochemistry*, Dover Publications.
3. J. O. M. Bockris, A. K. N. Reddy, *Modern Electrochemistry, Vol. I and II*, Kluwer Academic / Plenum Publishers, 2000.

#### **MODULE V *Surface Chemistry and Colloids* (10 h)**

Langmuir's unimolecular theory of adsorption, Adsorption isotherms, BET equation, derivation, determination of surface area of adsorbents, heat of adsorption and its determination. Gibbs adsorption isotherm. Colloids: Colloidal surfactants, classification – cationic, ionic and ionogenic surfactants. Micelles - causes of micellar formation. Micelle structure. Determination critical micellar concentration stabilizing action of surfactants. Practical importance of colloidal surfactants - Tannins and dyes.

#### **MODULE VI *Photochemistry* (8 h)**

Radiative and non-radiative transitions - chemiluminescence photoluminescence, cathodoluminescence, electroluminescence, bioluminescence, thermoluminescence, fluorescence, theory of fluorescence, stokes antistokes and resonance fluorescence - photosensitization - sensitised fluorescence - quenching of fluorescence. Theory of quenching of fluorescence. Principles of utilization of solar energy- solar cells.

##### **References**

1. F. Daniels, R. A. Alberty, *Physical Chemistry*, 5th Edn., Wiley Eastern, 1980.
2. S. Glasstone, *Physical Chemistry*, Mac Millan and Company, 1962.
3. G. Raj, H. Misra, *Photochemistry*, Goel Publishing House.
4. P. W. Atkins, *Physical Chemistry*, 6th Edn., Oxford University Press, 1998.
5. C. H. Dupeg, R. L. Chapman, *Molecular Reactions and Photochemistry*, Prentice Hall.
6. Cox, Kemp, *Introductory Photochemistry*, McGraw Hill.
7. P. Suppan, *Chemistry and Light*, RSC London.

#### **MODULE VII *Nuclear and Radiation Chemistry* (14 h)**

Nuclear binding energy, semi empirical mass equation, stability rules, magic numbers, nuclear models, shell, liquid drop, fermi gas, collective and optical models. Nuclear reactions: Types, conservation, reaction cross section, compound nucleus theory, specific nuclear reactions, photonuclear and thermonuclear reactions.

Nuclear fission- theory of fission - spontaneous and induced fission - neutron capture cross section and critical size, principle and working of nuclear power plants. Nuclear fusion. Neutron activation analysis.

Radiation chemistry - interaction of radiation with matter - processes responsible for energy loss, range and range energy relation. Methods of detection and measurement of radiation. Physical

and chemical radiation effects in solids. Radiation chemistry of water and aqueous ferrous sulphate solution. Dosimetry..

#### References

1. Friedlander, J. W. Kennedy, *Introduction to Radiochemistry*, John Wiley and Sons, 1981.
2. S. Glasstone, *Source Book on Atomic Energy*, 3rd Edn., Affiliated East-West Press Pvt. Ltd., 1967.
3. H. J. Arnikar, *Essentials of Nuclear Chemistry*, 4th Edn., New Age International, New Delhi, 1995.
4. J. B. Rajam, *Atomic Physics*, S. Chand and Co. Pvt. Ltd., 1974.
5. Friedlander, J. W. Kennedy, J. M. Miller, *Nuclear and Radiochemistry*, 3rd Edn., John Wiley and Sons, 1981.
6. J. W. T. Spinks, R. J. Woods, *An introduction to Radiation Chemistry*, John Wiley and Sons, 1964.

#### MODULE WISE WEIGHTAGE FOR QUESTIONS

| MODULE | WEIGHTAGE |
|--------|-----------|
| I      | 8         |
| II     | 6         |
| III    | 7         |
| IV     | 7         |
| V      | 7         |
| VI     | 10        |
| VII    | 5         |

**PC2 C 06 THEORETICAL CHEMISTRY II Credits: 4****MODULE I *Molecular Symmetry and Mathematical Groups* (10 h)**

Symmetry elements and symmetry operations in molecules, Complete set of symmetry operations of a molecule, Point groups and their systematic identification. Mathematical group, Finite and infinite group, Abelian and Cyclic groups. Group multiplication table. Classes in a group, Similarity transformation. Matrix algebra, Addition and multiplication of matrices, Inverse of a matrix, Square matrix, Character of a matrix, Diagonal matrix, Direct product and direct sum of square matrices, Block diagonalized matrix, Solving linear equations by the method of matrices. Matrix representation of symmetry operations.

**MODULE II *Theory of Molecular Symmetry* (10 h)**

Representation of groups, Basis for a representation, Representations using vectors, atomic orbitals and Cartesian coordinates positioned on the atoms of molecule (H<sub>2</sub>O as example) as the basis, Reducible and irreducible representations, Construction of irreducible representation by reduction (qualitative demonstration only), Great orthogonality theorem (GOT) (no derivation), Construction of irreducible representation using GOT, Construction of character tables (C<sub>2</sub>V, C<sub>3</sub>V, C<sub>2</sub>h and C<sub>4</sub>V as examples), Nomenclature of irreducible representations-Mulliken symbols, Symmetry species. Derivation of reduction formula using GOT, Reduction of reducible representations, (e.g., G<sub>cart</sub>) using the reduction formula, Direct sum and direct product of irreducible representations. Connection between group theory and quantum mechanics.

**MODULE III *Applications of Group Theory - I* (10 h)**

- i) Vanishing and non-vanishing integrals. Transition moment integral and selection rules. Overlap integrals and conditions for overlap.
- ii) MO treatment of H<sub>2</sub>O, Classification atomic orbitals involved into symmetry species, Group orbitals, Symmetry adapted linear combination (SALC), Projection operator, Construction of MOs, Electronic configuration of H<sub>2</sub>O, Symmetries of the ground and excited states, Electronic transitions and selection rules, Laporte selection rule for centro symmetric molecules.

**MODULE IV *Applications of Group Theory- II* (10 h)**

- i) Treatment hybridization in BF<sub>3</sub> and CH<sub>4</sub>, Inverse transformation and construction of hybrid orbitals.
- ii) Molecular vibrations, Symmetry species of normal modes of vibration, Construction of G<sub>cart</sub>. Normal coordinates and drawings of normal modes (e.g., H<sub>2</sub>O and NH<sub>3</sub>), Selection rules for IR and Raman activities, Complementary character of IR and Raman Spectra, Determination of IR active and Raman active modes of molecules (e.g., H<sub>2</sub>O, NH<sub>3</sub>, CH<sub>4</sub>, SF<sub>6</sub>).

**MODULE V (11 h)**

- i) *General Theory of Spectra*

Electromagnetic radiation and its different regions, Interaction of matter with radiation and its effect on the energy of the molecule. Origin of molecular spectra, Theory of the origin of rotational, vibrational and electronic spectra. Intensity of spectral lines, Dependence of intensity on population, transition probabilities,

Transition moment integral, Selection rules. Line widths, Doppler broadening, Lifetime broadening.

*ii) Microwave Spectroscopy*

Rotation spectra of diatomic and polyatomic molecules, Rigid and non-rigid rotator models, Asymmetric, symmetric and spherical tops. Isotope effect on rotation spectra, Stark effect, Nuclear and electron spin interactions. Rotational transitions and selection rules. Microwave spectrometer – Principles & Instrumentation.

Applications.

*iii) Vibrational Spectroscopy*

Vibrational spectra of diatomic and polyatomic molecules, Harmonic oscillator model, Anharmonicity, Vibrational transitions and selection rules. Morse potential, Fundamentals, Overtones, Hot bands, Combination bands, Difference bands.

**MODULE VI (11 h)**

i) Vibration-rotation spectra of diatomic and polyatomic molecules, P, Q, R branches. IR and FTIR spectrophotometer - Principles & Instrumentation, Applications.

*ii) Raman Spectroscopy*

Pure rotational, pure vibrational Raman spectra, Vibrational-rotational Raman spectra, Selection rules, Mutual exclusion principle.

Raman spectrophotometer- Principles & Instrumentation, Laser Raman spectroscopy, Applications.

*iii) Electronic Spectroscopy*

Basic principles, Beer - Lambert law, Molar extinction coefficient, Intensity of electronic transitions. Types of electronic transitions. Franck - Condon principle, Ground and excited electronic states of diatomic molecules. Electronic spectra of polyatomic molecules, Chromophores. The fate of electronically excited state species- Vibrational relaxation, External conversion, Internal conversion, Fluorescence, Phosphorescence. Jablonski diagram. Electronic spectra of conjugated molecules - dissociation and predissociation spectra.

UV-Visible spectrophotometer - Principles & Instrumentation. Applications.

**MODULE VII (10 h)**

*i) NMR Spectroscopy*

Magnetic properties of nuclei, Theory and measurement techniques, Solvents used, Chemical shift and factors influencing chemical shift, Shielding effects, Spin-spin interaction, Coupling constant, Factors influencing coupling constant, Effects of chemical exchange, Fluxional molecules, Hindered rotation on NMR spectrum, Karplus's relationships, NMR spectrometer- Principles and instrumentation. Multiple NMR spectroscopy (brief account). Applications of NMR spectroscopy to structure elucidation of simple organic and inorganic molecules. FT NMR.

*ii) ESR Spectroscopy*

Theory and measurement techniques, Hyperfine interactions, Equivalent and nonequivalent protons, Kramer's theorem. ESR spectrometer- Principles and instrumentation. Applications in structure elucidation of simple molecules.

*iii) Mossbauer spectroscopy*

The Moss Bauer effect. Instrumentation. Hyperfine interactions, isomer shift, electric quadruple and magnetic hyperfine interactions. Applications.

*iv) Mass Spectrometry*

Basic principles, Instrumentation - Mass spectrometer, interpretation of mass spectra, resolution, exact masses of nuclides, molecular ions, isotope ions. Fragmentation processes - McLafferty rearrangements, retro Diels - Alder fragmentation. Application in structure elucidation and evaluation of heats of sublimation and ionization potential.

**References**

1. F. A. Cotton, *Chemical applications of Group Theory*, 2nd Edn., Wiley Eastern, 1971.
2. Jaffe, Orchin, *Symmetry in Chemistry*, Wiley Eastern.
3. L. H. Hall, *Group Theory and symmetry in Chemistry*, McGraw Hill
4. R. McWeeny, *Symmetry: An Introduction to Group Theory and its Applications*, Pergamon Press, London, 1963.
5. P. H. Walton, *Beginning Group Theory for Chemistry*, Oxford University Press Inc., New York, 1998.
6. A. W. Joshi, *Elements of Group Theory for Physicists*, New Age International Publishers, 1997.
7. P. W. Atkins, *Physical Chemistry*, 6th Edn., Oxford University Press, 1998.
8. F. Daniels, R. A. Alberty, *Physical Chemistry*, 5th Edn., Wiley Eastern, 1980.
9. D. A. Mc Quarrie, J. D. Simon, *Physical Chemistry, A Molecular Approach*, University Science Books, 1997.
10. K. J. Laidler, J. H. Meiser, B. C. Sanctuary, *Physical Chemistry*, Houghton Mifflin Company, New York, 2003.
11. C. N. Banwell, *Fundamentals of Molecular Spectroscopy*, Tata McGraw Hill, New Delhi, 1994.
12. G. M. Barrow, *Introduction to Molecular Spectroscopy*, McGraw Hill, 1962.
13. H. H. Willard, L.L. Merritt, J. A. Dean, *Instrumental Methods of Analysis*, 4th Edn., Affiliated East-West Press Pvt. Ltd., 1965.
14. N. Sathyanarayana, *Electronic Absorption Spectroscopy and Related Techniques*, University Press, 2000.
15. R. S. Drago, *Physical Methods in Inorganic Chemistry*, Affiliated East-West Press Pvt. Ltd., 1977.

**MODULE WISE WEIGHTAGE FOR QUESTIONS**

| MODULE | WEIGHTAGE |
|--------|-----------|
| I      | 7         |
| II     | 7         |
| III    | 7         |
| IV     | 7         |
| V      | 7         |
| VI     | 8         |
| VII    | 7         |

## **SYLLABUS - PRACTICAL COURSES ( I & II Semesters)**

### **PC1 & PC2 P 01 INORGANIC CHEMISTRY Credits: 4**

#### **MODULE I**

Separation and identification of four metal ions of which two are less familiar elements like W, Se, Te, Mo, Ce, Th, Ti, Zr, V, U and Li. (Eliminating acid radicals not present). Confirmation by spot tests.

#### **MODULE II**

Volumetric Determinations using:

- a) EDTA (Al, Ba, Ca, Cu, Fe, Ni, Co, hardness of water, etc.)
- b) Estimations, involving quantitative separation of suitable binary mixtures of ions  $\text{Cu}^{2+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Fe}^{3+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Ca}^{2+}$ ,  $\text{Mg}^{2+}$ ,  $\text{Cr}_2\text{O}_7$
2. Ba, Ag, etc. in solution by volumetric, gravimetric, colorimetric and electroanalytical methods.
- c) Analysis of ores and alloys like dolomite, galena, ilmenite, monazite, feldspar and kaoline and two alloys.

#### **MODULE III**

Colorimetric determination of chromium, iron, manganese, nickel, and titanium using either Dubosque or photoelectric colorimeter.

#### **References**

1. G.H. Jeffery, J. Bassett, J. Mendham, R. C. Denny, *Vogel's Text book of Quantitative Chemical Analysis*, 5th Edn., ELBS, 1989.
2. D A Skoog, D M West, *Analytical Chemistry, An Introduction*, 4th Edn., CBS Publishing Japan Ltd., 1986.
3. E. J. Meehan, S. Bruckenstein, I. M. Kolthoff, E. B. Sandell, *Quantitative Chemical Analysis*, 4th Edn., The Macmillan Company, 1969.
4. R. A. Day (Jr), A. L. Underwood, *Quantitative Analysis*, 6th Edn., Prentice Hall of India, 1993.

### **PC1 & PC2 P 02 ORGANIC CHEMISTRY Credits: 4**

#### **MODULE I Laboratory Techniques**

Methods of separation and purification of organic compounds - fractional, steam and low-pressure distillations, fractional crystallisation and sublimation

#### **MODULE II Qualitative Organic Analysis**

Separation and identification of the components of organic binary mixtures (at least ten) by semimicro analytical techniques. Determination of M.P/B.P of the separated components. Separation of organic mixtures using paper, thin layer and column chromatography. Determination of  $R_f$  value.

#### **MODULE III Organic Preparations**

Preparation of about fifteen organic compounds (at least six double stage- including photochemical reactions) illustrating important synthetic methods and reactions such as Friedel-Crafts reaction, Grignard, Perkin, Reimer-Tiemann, Sandmeyer, and Cannizzaro reactions, Claisen, Aldol, and benzoin condensations. Selective reduction in polynitro aromatic compounds; diazocoupling, phthalein fusion, etc.

#### **MODULE IV *Quantitative Organic Analysis.***

Estimation of nitrogen by Kjeldahl method, estimation of hydroxyl and carbonyl groups, determination of iodine number and saponification value of oils. Estimation of reducing sugar, amines, phenols, esters, vitamins (A and C), drugs (aspirin, paracetamol).

#### **References**

1. B. S. Furnis, A. J. Hannaford, P. W. G. Smith, A. R. Tatchell, *Vogel's Textbook of Practical Organic Chemistry*, ELBS/Longman, 1989.
2. Fieser, *Experiments in Organic Chemistry*.
3. Mann, Saunders, *Practical Organic Chemistry*, 1957.
4. Dey, Sitaraman, Govindachari, *A Laboratory Manual of Organic Chemistry*, 3rd Edn., 1957.
5. Cheronics an Patrikin *Semi-micro Organic Analysis*.
6. A. J. Vogel, *Qualitative Organic Analysis*.
7. P. R Singh, D. C Gupta, K. S. Bajpal, *Experimental Organic Chemistry, Vol. I and II*, 1980.
8. R. Srinivasan, Ed. *Photochemical Synthesis, Vol. I and II*.

### **PC1 & PC2 P 03 PHYSICAL CHEMISTRY Credits: 4**

#### **MODULE I *Colligative Properties***

1. Molecular weight from depression by transition method- cooling curve method.
2. Molecular weight by cryoscopic method.
3. Molecular weight Rast method.

#### **MODULE II *Viscosity***

1. Determination of viscosity of pure liquids (water, methanol, ethanol, glycerol, benzene, nitrobenzene, carbon tetrachloride).
2. Determination of composition of binary liquid mixtures (benzene-nitrobenzene, water-alcohol).
3. Determination of molecular weight of a polymer (polystyrene in toluene).

#### **MODULE III *Conductivity Experiments***

1. Equivalent conductance of a weak acid- verification of Ostwald's dilution law calculation of dissociation constant.
2. Equivalent conductance of strong electrolytes (KCl). Verification of Onsagar equation.
3. Activity coefficient of Zn in 0.002M ZnSO<sub>4</sub> using Debye-Huckel limiting law.
4. Solubility product of a sparingly soluble salt (e.g., AgCl, BaSO<sub>4</sub>)
5. Conductometric titrations
  - (a) HCl vs NaOH
  - (b) (HCl + CH<sub>3</sub>COOH) vs NaOH
  - (c) AgNO<sub>3</sub> vs KCl.

#### **MODULE IV *Potentiometry***

1. Electrode potentials of Zn and Ag electrodes in 0.1 M and 0.001 M solutions at 25 °C and determination of standard potentials.
2. Mean activity coefficient of an electroanalyte at different molalities by EMF method.
3. Dissociation constant of acetic acid by potentiometric titration.

4. Determination of strength of the given HCl solution by differential potentiometric titration.
5. Dissociation constant of acetic acid in DMSO, DMF, acetone and dioxane by titrating with NaOH.
6. Potentiometric titration.
  - i) Mixture of chloride and iodide.
  - ii) Mixture of HCl and CH<sub>3</sub>COOH.

#### **MODULE V Chemical Kinetics**

1. Specific reaction rate of acid catalysed hydrolysis of methyl acetate.
2. Temperature coefficient and energy of activation of hydrolysis of methyl acetate.  
Determination of Arrhenius parameters.
3. Saponification of ethyl acetate (titration/conductance method).
4. Inversion of cane sugar in presence of HCl by polarimetry.
5. Iodination of acetone- determination of order.

#### **MODULE VI Adsorption** (3 experiments)

1. Verification of Freundlich and Langmuir adsorption isotherms.
2. Determination of concentration of acetic acid/oxalic acid using Freundlich and Langmuir adsorption isotherms.

#### **MODULE VII Phase Equilibria**

1. Phase diagram of a simple eutectic system.
2. Phase diagram of a binary solid system forming a compound.
3. Phenol-water system, aniline-water system.
4. Ternary liquid system with one pair of partially miscible liquids (DMSO-benzene-water, acetone-chloroform-water, etc.).

#### **References**

1. A. Finlay, J. A. Kitchener, *Practical Physical Chemistry*, Longman.
2. A. M. James, *Practical Physical Chemistry*, J. A. Churchill Ltd., 1961.
3. F. Daniel, J. W. Williams, P. Bender, R. A. Alberty, C. D. Cornwell, J. E. Harriman, *Experimental Physical Chemistry*, McGraw Hill, 1970.
4. W. G. Palmer, *Experimental Physical Chemistry*, 2nd Edn., Cambridge University Press, 1962.
5. D. P. Shoemaker, C. W. Garland, *Experimental Physical Chemistry*, McGraw Hill.



**UNIVERSITY OF CALICUT**  
**M. Sc. POLYMER CHEMISTRY- SEMESTER III**  
**PC3 C 07 INORGANIC CHEMISTRY- II Credits: 4**

**MODULE I (9 h)**

Electronic spectra of complexes. Terms of  $d^n$  configurations, selection rules. Effect of ligand field on RS terms. Orgel diagram and its uses. Calculation of  $Dq$ ,  $B$  and  $\beta$  parameters. Tanabe-Sugano diagrams. Charge transfer transition, spectra of lanthanides. Magnetic properties of metal complexes – types of magnetic behaviour, paramagnetism- the Curie and Curie-Weiss law.  $\mu_J$ ,  $\mu_L+S$  and  $\mu_{spin}$ -only expressions, quenching of orbital magnetic moment, spin-orbit coupling, magnetic properties of lanthanides, antiferro magnetic interactions, determination by Gouy method.

**MODULE II (9 h)**

Reaction mechanisms of metal complexes- classification, substitution reactions in octahedral complexes. A, D and I mechanisms, aquation and base hydrolysis. The Eigen-Wilkins Mechanism. Fuoss-Eigen equation. Aquation and base hydrolysis mechanism Substitutions in square planar complexes. Substitution reactions in square planar complexes. The trans effect-Applications and theories of trans effect, The cis effect. Redox reaction mechanism, inner and outer sphere mechanisms, Marcus theory, photochemical reactions of metal complexes.

**MODULE III (8 h)**

Infrared spectra of metal complexes. Changes in ligand vibrations on coordination– metal ligand vibrations. CD- and ORD spectra of metal complexes. ESR spectra - application to copper complexes, Mossbauer spectra - application to iron complexes.

**MODULE IV (15 h)**

i) Organometallic compounds- Classification and nomenclature, alkyls and aryls of main group metals, structural types, metal carbenes and carbenes. The 18-electron rule, syntheses, structure and bonding in metal carbonyls. Synthesis, structure, reactions and bonding in metal complexes of ethylene, allyl, butadiene, acetylene.

ii) Synthesis, structure, bonding and reactions of complexes of  $C_4H_4$ ,  $C_5H_5$  (iron group),  $C_6H_6$  (chromium group).

*Fluxional Organometallics*

Metal-metal bond and metal clusters- structure and bonding in halide clusters and higher carbonyl clusters. Metal complexes of  $H_2$ ,  $N_2$ ,  $O_2$  and  $NO$ - structure and bonding.

**MODULE V (8 h)**

Applications of organometallic compounds in organic synthesis and catalysis oxidative addition, reductive elimination and insertion reactions. Carbonylation by Collman's reagent. Hydrogenation, hydroformylation and polymerization of alkenes using organometallic catalysts. Monsanto acetic acid process, Wacker process.

**MODULE VI (9 h)**

Introduction to bioinorganic chemistry, occurrence of elements in biological systems, bulk and trace metal ions, coordination sites of biologically important ligands. Metalloenzymes- cytochrome P450, peroxidase, superoxide dismutase, cytochromes, vitamin B12. Oxygen transport- hemoglobin and myoglobin, storage and transport of metal ions- Ferritin, transferring. Biological nitrogen fixation, Chlorophyll- photosystem I and II. Platinum complexes as anticancer drugs.

**References**

1. F. A. Cotton, G. Wilkinson, C. A. Murillo, M. Bochmann. *Advanced Inorganic Chemistry*, John Wiley & Sons, 1999.
2. J. E. Huheey, E. A. Keiter, R. L. Keiter, *Inorganic Chemistry, Principles Structure and Reactivity*, Pearson, 2001.
3. H. J. Emeleus, A. G. Sharp, *Modern Aspects of Inorganic Chemistry*.
4. P. Powell, *Principles of Organometallic Chemistry*, 2nd Edn., ELBS, 1988.
5. R. C. Mehrotra, A. Singh, *Organometallic Chemistry, A Unified Approach*, Wiley Eastern, 1991.
6. K. F. Purcell, J. C. Kotz, *Inorganic Chemistry*.
7. S. F. Kettle, *Coordination Compounds*.
8. Sutton, *Electronic Spectra of Coordination Compounds*.

#### **UNIT VII Instrumental Methods of Analysis (12 h)**

Electroanalytical techniques: Voltammetry, cyclic voltammetry, polarography, amperometry, coulometry, conductometry, spectrophotometry. Thermal analysis: Principles, TG, DTA and DSC- their applications, polarimetry, refractometry, chromatography- column, paper, TLC., Gas and HPLC. Determination of  $R_f$  value. Principles of atomic absorption spectroscopy (AAS) and atomic emission spectroscopy (AES), solvent extraction and ion exchange methods, light scattering techniques including nephelometry.

#### **References**

1. G. H. Jeffery, J. Bassett, J. Mendham, R. C. Denny, Vogel's Text book of Quantitative Chemical Analysis, 5th Edn., ELBS, 1989.
2. Williard, Merrit, Dean Instrumental, *Methods in Chemistry*.
3. Skoog, West and Holler, *Fundamentals of Analytical Chemistry*, 8th Edn., Thomson and Brooks, 2004.
4. R. S. Drago, *Physical Methods in Inorganic Chemistry*.

#### **UNIVERSITY OF CALICUT**

#### **M.Sc. POLYMER CHEMISTRY– SEMESTER III**

#### **PC3 C08 PHYSICAL CHEMISTRY II Credits 4**

#### **MODULE I Statistical Mechanics- I (8 h)**

Basic principles, permutations, probability distribution of particles in energy states. Microstates and macrostates (configurations). Statistical weight factor ( $g$ ), Most probable distribution- Boltzmann distribution law. The partition function and its relation to the thermodynamic functions.

#### **MODULE II Statistical Mechanics- II (5 h)**

##### **i) The Perfect Gas**

Factorisation of the partition function into translational, rotational, vibrational and electronic parts. The corresponding contributions to the thermodynamic properties. The anomalous heat capacity- temperature relation for hydrogen- *ortho* and *para* hydrogen.

##### **ii) The atomic crystal- Einstein's theory of atomic crystals- Debye's modification.**

#### **MODULE III Statistical Mechanics- III (12 h)**

i) The imperfect gases- The virial expression and the virial coefficients- relation between the virial coefficients and the cluster integrals.

ii) The ideal Fermi gas- Fermi- Dirac distribution law- Equation of state of an ideal Fermi gas- limiting forms of the expression at (a) high temperatures and low densities (b) low temperature and high densities. Application to electrons in metals.

iii) The ideal Bose gas

The Bose- Einstein distribution law. Application to Bose- Einstein condensation. Application to liquid helium.

#### **References (MODULES I, II & III)**

- 1 G. S. Rush Brooke, *Statistical Mechanics*, Oxford University Press.
- 2 T. L. Hill, *Introduction to Statistical Thermodynamics*, Addison Wesley.
- 3 K. Huary, *Statistical Mechanics, Thermodynamics and Kinetics*, John Wiley.
- 4 O. K. Rice, *Statistical Mechanics, Thermodynamics and Kinetics*, Freeman and Co.
- 5 F. C. Andrews, *Equilibrium Statistical Mechanics*, John Wiley and sons, 1963.

#### **MODULE IV Chemical Kinetics– I (12 h)**

- i) Theory of reaction rates - Arrhenius theory, collision theory and transition state theory. Significance of Arrhenius parameters - theoretical calculation of the activation energy - potential energy surfaces - London equation. A comparative study of collision and transition state theories. Theories of unimolecular reactions.
- ii) Kinetics of reactions involving reactive atoms and free radicals. Rice – Herzfeld mechanism and steady state approximation in the kinetics of organic gas phase decompositions. Kinetics of chain reactions - branching chain and explosion limits.

#### **MODULE V Chemical Kinetics– II (14 h)**

- i) Catalysis - Theories of general and specific acid - base catalysis - enzyme catalysis- Michaelis Menten equation - heterogeneous catalysis - theory and principles - industrial applications.
- ii) Kinetics of reactions in solution - role of solvent in the kinetics of reactions - cohesive energy density of solvent and its influence on rates - effect of specific properties of solvent such as dielectric constant and dipole moment on rates of reactions between ions, dipoles and neutral molecules. Salt effect, primary and secondary salt effects: Fast reactions - study of the kinetics of fast reactions using relaxation time - Flash photolysis.

#### **References (MODULES IV & V)**

1. K. J. Laidler, *Chemical kinetics, Vol. I and II*, McGraw Hill.
2. A. A. Frost, R. J. Pearson, *Kinetics and Mechanism*, Wiley Eastern.
3. F. Daniels, R. A. Alberty, *Physical Chemistry*, 5th Edn., Wiley Eastern, 1980.
4. G. K. Vemulapalli, *Physical Chemistry*, Printice Hall of India.
5. D. A. McQuarrie, J. D. Simon, *Physical Chemistry, A Molecular Approach*, University Science Books, 1997.
6. K. J. Laidler, J. H. Meiser, B. C. Sanctuary, *Physical Chemistry*, Houghton Mifflin Company, New York, 2003.

#### **MODULE VI Introduction to Computers in Chemistry (7 h)**

Basic ideas of CPU, input and output devices, memory. Hardwares and softwares. System softwares and application softwares. Programming Languages: machine, assembly, high level languages. Interpreter and compiler. Flow charts and Algorithms. Introduction to BASIC language, BASIC characters, Numeric constants and variables, String variables, Symbols of arithmetic operations, Hierarchy of operations. BASIC Statements, User defined functions. Introduction to C language, C characters, Constants and Variables, C statements. C programming, Factorial of a number, Molecular weight of organic compounds. Basic ideas on the use of Internet in Chemistry Education.

#### **References**

1. J. B. Norton, *Introduction to BASIC*, BPB publishers.

2. S. M. Venit, *Programming in BASIC, Problem Solving with Structure and Style*, Jaico Publishing House, Bombay.
3. Madric, Donevan, *Understanding Computers*, McGraw Hill.
4. K. V. Raman, *Computers in Chemistry*, Tata McGraw Hill, 1993.
5. K. B. Wiberg, *Computer Programming for Chemists*, Benjamin Inc., NY, 1965.
6. N. Subramaniam, *Programming in Basic*, A.L. Wheeler and Co.
7. P. Lykose, *Personal Computers in Chemistry*, John Wiley and Sons, NY, 1981.
8. Ramesh Kumari, *Computers and Their Applications to Chemistry*, Narosa, New Delhi, 2002.
9. S. P. Singh, *Fundamentals of Computers*.
10. Bala Guruswamy, *Programming in BASIC*.
11. Yesharant Kanetkar, *Let Us C*, BPB Publishers.

#### **MODULE VII Introduction to Computational Quantum Chemistry (12 h)**

Review of Hartree-Fock SCF method, Electronic structure of molecules, The basis sets, STOs and GTOs, Nomenclature of basis sets. Semi-empirical and ab initio methods. Calculations using Gaussian Programme, Specification of molecular geometry using a) Cartesian coordinates and b) Internal coordinates, The Z-matrix, Z-matrices of some simple molecules (e.g., H<sub>2</sub>, H<sub>2</sub>O, Formaldehyde, Ammonia, Methanol), The structure of a Gaussian Input file.

#### **References**

- 1 D. A. McQuarrie, J. D. Simon, *Physical Chemistry, A Molecular Approach*, University Science Books, 1997.
- 2 I. N. Levin, *Quantum Chemistry*, 5th Edn., Pearson Education, Inc., 2000.
- 3 T. Clark, *A Handbook of Computational Chemistry*, John Wiley and Sons, Inc., 1985.
- 4 F. Jensen, *Introduction to Computational Chemistry*, John Wiley and Sons, 1999.

**UNIVERSITY OF CALICUT**  
**M.Sc. POLYMER CHEMISTRY– SEMESTER III**

***PC3 C09 POLYMER CHEMISTRY Credits: 4***

**MODULE I (10 h)**

Basic concepts of Polymer science, history, molecular weight and its distribution, synthetic and natural polymers. Classification as Plastics, rubbers, fibres, adhesives and coatings. Plastics- thermoplastics and thermosets, commodity, engineering and speciality plastics; Rubbers- general purpose and speciality rubbers, sources of monomers, polymerisability, stereochemistry, conformational analysis of polymers.

**MODULE II (8 h)**

Synthesis of high polymers, reactants for step growth polymerisation, vinyl monomers, step reaction (condensation) polymerization, mechanisms, kinetics and statistics, gelation.

**MODULE III (8 h)**

Radical chain (addition) polymerization, mechanisms of vinyl polymerization: initiation, propagation and termination. Kinetics of vinyl radical polymerization, degree of polymerization and chain transfer determination of individual rate constants, effects of temperature and pressure on chain polymerization.

**MODULE IV (9 h)**

Ionic and coordination chain (addition) polymerization, cationic polymerization, mechanisms, kinetics, anionic polymerization, mechanism, kinetics, coordination polymerization, Ziegler-Natta catalysis, mechanism of coordination polymerization- monometallic and bimetallic mechanisms. ring opening polymerization.

**MODULE V (10 h)**

Copolymerisation, kinetics, copolymer equation, monomer reactivity ratios evaluation, rate of copolymerisation, composition of copolymers, mechanisms, ionic copolymerisation, step reaction copolymerisation, block and graft copolymers.

**MODULE VI (15 h)**

i) Polymerisation conditions, comparison of polymerization systems, polymerization in homogeneous systems and heterogeneous systems, Smith-Ewart kinetics, solid phase polymerisation, polymerization reactors.

ii) Reaction of polymers, reaction with polyolefin's, polyenes, aliphatic pendant groups, aromatic pendant groups, cross-linking reactions, preparation of polymer derivatives.

**MODULE VII (10 h)**

Polymer degradation and stabilization: introduction, chemical degradation, physical degradation, photodegradation, thermal degradation, aging, degradation by microorganisms, biodegradable polymers- stabilisation, antioxidants. Polymer degradation kinetics.

**References**

1. F. W. Billmeyer, *Text Book of Polymer Science*, John Wiley and Sons.
2. R. B. Seymour, *Polymer Chemistry*, Marcel Dekker.

3. J. R. Fried, *Polymer Science and Technology*, Prentice Hall.

**UNIVERSITY OF CALICUT**  
**M.Sc. POLYMER CHEMISTRY– SEMESTER III**

**PC3 E01 POLYMER MATERIALS Credits: 4**

**MODULE I (9 h)**

Natural polymers: Proteins- Synthesis of peptides (solution and SPPS), structure of proteins, Nucleic acids- structure and synthesis in detail, lignins, cellulose, properties and applications, source, rubber latex, processing, dry rubber, technically specified and classified rubbers, modified forms of NR, reclaimed rubber, reclaiming processes.

**MODULE II (9 h)**

Structure, preparation, preparation and applications of polyolefins: polyethylene, LDPE, HDPE, LLDPE, chlorinated and chloro sulphonated polyethylene, ethylene copolymers, polypropylene, polypropylene copolymer, polyisobutylene, butyl rubber etc.

**MODULE III (16 h)**

i) Vinyl polymers; structure, preparation, properties and applications polystyrene, styrene based copolymers SAN, ABS, high impact polystyrene polyvinyl chloride, chlorinated PVC, vinyl chloride- vinyl acetate copolymer, poly(vinyl acetate) and its derivatives poly (vinyl alcohol), fluoro polymers; PTFE, PCTFE, PVF and PVDF, poly acrylics, PMMA, poly acrylonitrile, transformation into carbon fibre, polyacrylic acid.

ii) Diene polymers; structure preparation, properties and applications, polybutadiene rubber, styrene-butadiene rubber, oil extended SBR, thermoplastic elastomers from styrene-butadiene copolymers, nitrile rubber, polyisoprene, polychloroprene.

**MODULE IV (9 h)**

Polyesters: structure, preparation, properties and applications of thermoplastic polyesters, PET, PBT, thermoplastic polyester elastomers, polycarbonates, polyacrylates, liquid crystal polyesters, thermosetting polyesters, unsaturated polyesters, epoxy polymers.

**MODULE V (9 h)**

Polyamides and polyimide: structure, preparation, properties and applications, nylon 6, nylon 6,6 polyamide thermoplastic elastomers, aromatic polyamides, polyimides, modified polyimides, phenolics, novolacs and resoles, aminoplastic: UF & MF.

**MODULE VI (9 h)**

Silicon polymers; structure, preparation, properties and applications, silicon oils, silicon elastomers, polyurethanes, structure, preparation, properties and applications, thermoplastic polyurethane elastomers, polyurethane rigid and flexible foams.

**MODULE VII (9 h)**

Speciality polymers- thermally resistant polymers, fire resistance, hydrophilic polymers, polymers with electrical and electronic properties, ionic polymers, photoresists, polymers in non-linear optics, polymer in membrane separations.

**References**

1. D. Feldman, *Synthetic Polymers*, Chapman Hall, 1996.
2. R. Sinha, *Outlines Polymer Technology*, Prentice Hall India, 2000.
3. M. Morton, *Rubber Technology*.

**UNIVERSITY OF CALICUT**  
**M Sc POLYMER CHEMISTRY– SEMESTER IV**

***PC4 C10 PHYSICAL CHEMISTRY OF POLYMERS Credits: 4***

**MODULE I (14 h)**

Polymer chain structure and configuration, stereochemistry of repeating units, optical isomerism, geometrical isomerism. Solution properties, polymer conformation and chain dimensions, thermodynamics of polymer solutions, Flory-Huggins theory, Folry-Krigbaum and modified Flory-Huggins theory, phase equilibria, solubility parameter, intrinsic viscosity. Mark-Houwink equation.

**MODULE II (6 h)**

The amorphous state, conformation of the polymer chain, macromolecular dynamics. The Rouse-Bueche theory, Fickian and non-Fickian diffusions.

**MODULE III (10 h)**

The crystalline state, melting phenomena, crystal structure, unit cell, polyethylene and other polyolefin polymers, fringed micelle model, polymer single crystal spherulites, kinetics of crystallization. The Avrami equation, effect of chemical structure on the melting temperature and fibre formation.

**MODULE IV (9 h)**

Liquid crystalline polymers, liquid crystalline mesophases, phase diagrams, classification, lyotropic liquid crystalline chemical structure, thermotropic liquid crystalline structure, side chain liquid crystalline structure, thermodynamics and phase diagrams.

**MODULE V (15 h)**

Glass transition, dynamic mechanical behaviour through the five regions of viscoelastic behaviour, methods of measuring glass transition temperature (dilatometry, thermal methods, dielectric and magnetic methods), other transitions. Influence of time, temperature, and frequency on these relaxations. Theories of glass transition (free volume, kinetic and thermodynamic), effect of molecular weight and chemical structure on the glass transition temperature, damping.

**MODULE VI (6 h)**

Crosslinked polymers and rubber elasticity, rubber network structure, rubber elasticity concepts, thermodynamic equation of state. Mooney-Rivlin equation, Flory-Rehner equation.

**MODULE VII (10 h)**

Polymer viscoelasticity, introduction to the viscoelastic properties of polymers, Polymer viscoelasticity and rheology, stress relaxation and creep. Some simple linear viscoelastic models- Maxwell model, Voigt model, series combination of Maxwell and Voigt model, generalized linear viscoelasticity, the Boltzmann principle, the linear viscoelastic behavior of polymer solids, creep experiments, stress relaxation experiments, stress-strain experiments, oscillatory experiments, the elastic modulus, time temperature equivalence, time-temperature superposition principle. superposition principle.

5.4 Rheological properties of polymers-introduction to polymer melt

## References

1. P. C. Hiemenz, *Polymer Chemistry*, Marcel Dekker, New York.
2. L. H. Sperling, *Introduction to Physical Polymer Science*, Wiley Interscience.

## UNIVERSITY OF CALICUT

### M Sc POLYMER CHEMISTRY– SEMESTER IV

#### ***PC4 C12 TETING AND CHARACTERISATION OF POLYMERS Credits: 4***

##### **MODULE I (15 h)**

Standards and standards organizations, test methods and specifications, preparation of test pieces, conditioning, test methods for polymers and additives, density, polymer mol wt. Determination, cryoscopic determination and ebullioscopic method, vapour pressure method, osmotic pressure method, sedimentation velocity method, light scattering method, gel permeation chromatography.

##### **MODULE II (10 h)**

Mechanical properties of polymers, stress and strain, tensile properties, compressive properties, flexural properties, hardness, secant modulus, dynamic mechanical testing, torsion pendulum, DMA, rebound resilience impact, Charpy impact and falling weight, long term testing, creep, stress relaxation, friction and wear, abrasion testing.

##### **MODULE III (16 h)**

Electrical and optical properties, resistivity, dielectric strength, dielectric constant, dissipation factor, power factor, arc resistance, optical properties, light transmission, clarity, haze, reflectance, birefringence. Luminous transmittance

Thermal properties; thermal conductivity, heat capacity, thermal expansion, Vicat softening point, heat deflection temperature, T<sub>g</sub>, T<sub>m</sub> and other transitions. DTA, DSC, TGA, low temperature tests, brittleness test.

##### **MODULE IV (6 h)**

Flow properties of polymer melts and solutions, shear stress, shear rate, capillary rheometer, cone and plate rheometer.

##### **MODULE V (8 h)**

Spectroscopic characterization of polymers: IR spectroscopy, Raman spectroscopy, NMR spectroscopy, UV-visible, Fluorescence. X-ray diffraction, chemical methods and identification of polymers

##### **MODULE VI (5 h)**

Test on rubbers: Unvulcanized rubbers, PRI, scorch and cure rate vulcanized rubbers, heat ageing, flex cracking, heat build up.

##### **MODULE VII (10 h)**

Environmental resistance, effect of liquids, water absorption, effect of ozone, ozone cabinet, weathering, environmental stress cracking, biological attack, fire resistance, radiation resistance, gas, permeability.

## References

1. R. P. Brown, *Testing of Rubber*, Applied Science Publishers.
2. R. P. Brown, *Hand Book of Plastics Test Methods*.
3. Vishu Shah, *Handbook of Plastics Testing technology*, John Wiley and Sons, 1981.
4. Iyres, Mead, Rily, *Handbook of Plastics Test Methods*, Elite Publishers.



**UNIVERSITY OF CALICUT**  
**M Sc POLYMER CHEMISTRY– SEMESTER IV**

**PC4 C11 POLYMER TECHNOLOGY Credits: 4**

**MODULE I (12 h)**

Introduction to polymer processing, Importance of additives, plasticizers, fillers, stabilizers, flame retardants, colourants, antistatic agents and blowing agents. Principles of rubber compounding and thermostat compounding. Mixing machines.

**MODULE II (10 h)**

Extruders for plastics & rubbers, twin screw extruders, extrusion process, die swell and part dimension control, operating parameters, co-extrusion, Rubber injection moulding. extrudate defects like melt fracture, shark skin, alligator hide.

**MODULE III (8 h)**

Adhesives and surface coatings- concepts and terminology, Surface treatments, Mechanism of adhesion, mechanical interlocking, inter-diffusion, adsorption, surface reaction, electrostatic attraction. types of adhesives (hot melt, solutions, aqueous dispersion, activated adhesives, film adhesive, pressure sensitive adhesives, polymerising types, radiation curable. theories of bonding, bonding and testing, pigments and paints, paint properties and their evaluation.

**MODULE IV (10 h)**

Polymer blends-importance, plastic-plastic, rubber and plastics-rubber blends miscibility and compatibility, methods of determining miscibility and compatibility, compatibilizing agents, processing of polymer blends.

**MODULE V (10h)**

Introduction to composite materials-classification-advantages polymer composites, reinforcement fibres-glass, carbon, Kevlar, boron, SiC-composition, manufacture surfacetreatment of glass fibres-coupling agents.

**References**

1. M. Jones, *Polymer Processing*, Chapman and Hall.
2. W. C. Wake, *Adhesives and the Formulation of Adhesive*, Applied Science Publishers, London, 1976.
3. C. M. Blow, *Rubber Technology and Manufacture*.
4. D. R. Paul, S. Newman, *Polymer Blends*, Academic Press.
5. S. T. Peters (Ed.), *Handbook of Composites*, 2nd Edn. Chapman and Hill, 1998.
6. G Lubin, *Handbook of Composites*, VanNostrand, New York, 1993.

**UNIVERSITY OF CALICUT**  
**M Sc POLYMER CHEMISTRY– SEMESTER IV**

***PC3 E02 i) PLASTICS AND FIBRE TECHNOLOGY Credits: 4***

**MODULE I** Mixing and compounding (10 h)

Introduction to plastic processing, additives for plastics, mixing and compounding of plastics, mixing and compounding equipment.

**MODULE II** Moulding techniques I (10 h)

Plastic injection moulding , different types of injection moulding machines, details of injection moulding machine, injection moulding of thermosets. Extrusion, details of extruders, twin screw extruders, dies, post extrusion processing, calendering, laminating

**MODULE III** Moulding technique II (10 h)

Compression moulding: hydraulic presses, press capacity and pressure calculations, moulding process. Transfer moulding: moulding process, advantages. Blow moulding: extrusion and injection blow moulding. Rotational moulding: process and equipment. Reaction injection moulding: introduction, process and advantages.

**MODULE IV** Reinforced plastics (10 h)

Reinforced plastics: materials processing techniques viz- hand lay-up, spray lay up, filament winding autoclave and bag moulding.

**MODULE V** Fibre technology (10 h)

Fibers from cellulose and its derivatives, polyolefinic, polyester, polyamide, aramide carbon and glass fibers. Fiber spinning operations, different types of cords used in tyre industry, definition of denier, tex, tncity, different types of twisting, geo textiles.

**References**

1. C. J. Crawford, Plastic Engineering, Pergamon Press, London ,1999.
2. D. H. Morton, Polymer processing, Chapman and Hall, London, 1989.
3. George Mathews, Polymer mixing technology, Applied Science Publishers, London,1982.
4. Joel Frados (Ed) Plastic Engineering Hand book, Van Nostrand Reinhold Company, New York ,1976.

## **UNIVERSITY OF CALICUT**

### **M Sc POLYMER CHEMISTRY– SEMESTER IV**

#### ***PC4 E02 ii) POLYMER NANO TECHNOLOGY Credits: 4***

##### **MODULE I: Introduction (10h)**

Introduction to Nanotechnology with special emphasis on Nanocomposites: Composite material, Mechanical properties of Nano composite material: stress - strain relationship, toughness, strength, plasticity, Synthesis methods for various nanocomposite materials: sputtering, mechanical alloying, sol-gel synthesis, thermal spray synthesis.

##### **MODULE II: Classification of nanocomposites and nano fillers (10h)**

Ceramic-Metal Nanocomposites, Ceramic based nanoporous composite, Metal matrix nanocomposites, Polymer-based nanocomposites Carbon nanotube based nanocomposites and Natural nanobiocomposites, Biomimetic nanocomposites and Biologically inspired nanocomposites, Nano composites for hard coatings, DLC coatings, Thin film nanocomposites, Modeling of nanocomposites.

Classification of nano fillers – based on its origin and structure

##### **MODULE III: Processing of Nanocomposites (10h)**

Processing of polymer nanocomposites, properties of nanocomposites, Salt in filtration, Powder mixing, Intrusion method, Exfoliation & interaction, Gel-casting impregnation techniques: Hot melt impregnation, solution impregnation.

##### **MODULE IV: Evaluation & Testing of Nanocomposites (10h)**

Evaluation of mechanical properties of nanocomposites: Nano Indentation, Types of indentation: Oliver & Pharr, Joslin-Oliver, Vickers indenter process. Characterization techniques used to analyse the nano-fillers and nanocomposites XRD, Electron Microscopes, Scanning electron microscope, Modern transmission electron microscope, Scanning probe microscope-atomic force microscope, Scanning tunneling microscope, Self Assembly.

##### **MODULE V: Applications (10h)**

Application of nanocomposites in modern industry, medical field, homeland security, law enforcement, defense, structural and civil applications.

##### **References**

1. M. Balakrishna rao and K. Krishna Reddy, Encyclopaedia of Nanotechnology, Vol I to X Campus books.
2. HS Nalwa, Encyclopedia of Nanotechnology.
3. Lynn E. Foster, Nanotechnology – science, innovation and opportunity, Prentice Hall, Pearson education.
4. T. Pradeep, Nano: The Essentials – Understanding Nano Science and Nanotechnology, Tata McGraw Hill

**Text Books**

1. Charles P. Poole Jr and Frank J.Owens, Introduction to Nanotechnology, Wiley India Pvt Ltd.
2. WR Fahrner, Nanotechnology and Nano Electronics – Materials, devices and measurement techniques by , Springer publications
3. P.M. Ajayan, L.S. Schadler and P.V. Braun, Nanocomposite Science & Technology, Wiley-VCH GmbH Co.
4. P.Poole Jr and Frank J. Owens, Introduction to Nano Technology by Charles, Wiley India Pvt Ltd.
5. Mark Ranter, Daniel Ranter, Nanotechnology, A gentle introduction to the next big idea, Pearson education

**UNIVERSITY OF CALICUT**  
**M Sc POLYMER CHEMISTRY– SEMESTER IV**  
**PC4P04POLYMERCHEMISTRYPRACTICALSI**

**PART I: Preparation of Polymers**

Any six preparations of the following (preparations are only illustrative, same or similar may be carried out):

01. Preparation of nylon -6,6 (Interfacial polycondensation)
02. Preparation of PMMA (free radical bulk polymerization)
03. Preparation of polyacrylamide (free radical polymerization)
04. Preparation of polyacrylamide (redox polymerization)
05. Preparation of glyptal resin
06. Preparation of linear polystyrene (free radical polymerization)
07. Preparation of crosslinked polystyrene (suspension polymerization)
08. Preparation of phenol formaldehyde resin (resoles and novolacs)
09. Preparation of urea formaldehyde resin
10. Preparation of polyaniline
11. Preparation of aniline formaldehyde resin

**PART II**

Determination of filler content in compounded polymers.

**PART III**

**References**

01. E.A. Collins, J. Bares, F.W. Billmeyer, Experiments in Polymer Science, Wiley-Interscience, 1973.  
57
02. S.H. Pinner, A Practical Course in Polymer Chemistry, Pergamon, 1961.
03. D. Braun, H. Cherdron, W. Kern, Practical Macromolecular Organic Chemistry, 3<sup>rd</sup> Edn, Harwood Academic Pub., 1984.
04. S.R. Sandler, W. Karo, Polymer Synthesis, Vol.1, Academic Press, 1992.
05. S.R. Sandler, W. Karo, Polymer Synthesis, Vol.2, Academic Press, 1993.
06. S.R. Sandler, W. Karo, Polymer Synthesis, Vol.3, Academic Press, 1998.
07. D. C. Blackley, Polymer Latices, Vol.1, 2 & 3, 2<sup>nd</sup> Edn., Springer, 1997.
08. W.C. Wake, Analysis of Rubbers and Rubber like Polymers, 2<sup>nd</sup> Edn, Wiley-Interscience, 1969.

PC4 P05

**PART I: Latex Analysis**

01. Determination of total solid content of latex
02. Determination of alkalinity of latex
03. Determination of dry rubber content of latex
04. Determination of volatile fatty acid number of latex
05. Determination of viscosity of latex
06. Determination of KOH number