DEPARTMENT OF CHEMISTRY

M.Sc. - Chemistry

SYLLABUS

Effective from the Academic Year 2016-2017

LOYOLA COLLEGE (Autonomous)

Ranked 2 in INDIA RANKING 2017 - NIRF

'College of Excellence' Status Conferred by UGC in 2014

Re-accredited with 'A' Grade (3.70 CGPA) by NAAC in 2013

Chennai - 600 034

RESTRUCTURING-2016 (2016-17 batch ONWARDS)
PG - Arts / Science / Commerce / Social Work

Part	Semester 1	Semester 2	Summer Vacation	Semester 3	Semester 4	Total Hours
Major Core (MC)	30(20 C)	24(20 C)	– –	20(15 C)	30(24 C)	104(79 C)
Elective Subject (ES)	– –	4(3 C)	– –	4(3 C)	– –	8(6 C)
Inter - Disciplinary (ID)	– –	– –	– –	6(5 C)	– –	6(5 C)
Self study Paper (SSP)				Outside class hours(2C)		(2 C)
Summer Training Program (STP)	– –	– –	3 to 4 weeks (1 C)	– –	– –	(1 C)
Life Skills Training (LST)	– –	2h + 2h# (2 C)	– –	– –	– –	2+2# (2 C)
Extension Activities	LEAP	LEAP(3 C)	– –	– –	– –	(3 C)
Total Hours (Total Credits)	30 (20 C)	30+2# (23+5 C)	--(1 C)	30 (23+2 C)	30 (24 C)	120+2# (90+6+2*)C

Note: A theory paper shall have 5 to 6 contact hours and a practical session shall have 3 to 5 contact hours.

New format of the subject codes from the 2016 regulation

Subject codes are 10 characters long:

1st	2nd	3rd	4th	5th	6th	7th	8th	9th	10th

- 1st & 2nd digits – last two digits of regulation year in YY format (If 2016, it will be 16).
- 3rdalphabet: U – UG / P – PG / M – M.Phil. / D – Ph.D.
- 4th & 5thalphabets: department wise program code(example – MT / CO / HT…..)
- 6th digit: Semester for UG/ PG / M.Phil. and year for Ph.D.
- 7th & 8th alphabet: Category of paper or group of category of papers (GE/RL/OL/HE/OR/AL /ES/SK/MS/CM/CC/ ……)
- 8th & 9th digits: subject number range (01 to 99).

For example,

Example 1:16UCH1MC01

16 – Admitted in 2016
U – UG student
CH – Chemistry Student
1 – 1st Semester subject
MC01 – Major paper

Example 2:16PCO2ID01

16 – Admitted in 2016
P – PG student
CO – Commerce Student
2 – 2nd Semester subject
ID01 – Inter disciplinary paper

- For subjects which are carried forward from one regulation to the next, the first two digits representing the regulation alone will change.
- Subjects which are not carried forward from one regulation to the next, will not appear in the new regulation.
- For new subjects which need to be added to a regulation, a new subject code must be created in continuation of the last created code under that type/category.
- Subject codes which are identical (except for the first two digits which represent the regulation year) are treated as equivalent for the purpose of syllabus / question paper setting / conducting examination / etc.

M.Sc. Chemistry (Shift - I)

(WITH EFFECT FROM 2016-2017 BATCH)

Sl. No	Sub. Code No.	Title of the paper
1	16PCH1MC01	Organic Reaction Mechanism and Stereochemistry
2	16PCH1MC02	Concepts in Inorganic Chemistry
3	16PCH1MC03	Quantum Chemistry and Group Theory
4	16PCH1MC04	Analytical Chemistry
5	16PCH1MC05	Organic laboratory techniques-I
6	16PCH1MC06	Inorganic quantitative analysis and preparations
7	16PCH2MC01	Organic Reaction Mechanism and Heterocyclic compounds
8	16PCH2MC02	Coordination Chemistry
9	16PCH2MC03	Molecular Spectroscopy
10	16PCH2MC04	Organic laboratory techniques -II
11	16PCH2MC05	Inorganic semimicro qualitative analysis
12	16PCH2ES01	Biomolecules and Natural Products
13	16PCH2ES02	Surface Chemistry and Catalysis
14	16PHE2FC01	Life Skills Training
15	16PCH3MC01	Main Group Elements and Nuclear Chemistry
16	16PCH3MC02	Thermodynamics and Chemical Kinetics

17	16PCH3MC03	Scientific Research Methodology & Communications
18	16PCH3MC04	Physical Chemistry Practical-I
19	16PCH3ES01	Physical Concepts in Inorganic Chemistry
20	16PCH3ES02	Applied Organic Chemistry
21	16PCH3TP01	Summer Training Programme
22	16PCH3ID01	Materials Science
23	16PCH4MC01	Organic Synthesis and Photochemistry
24	16PCH4MC02	Electrochemistry
25	16PCH4MC03	Physical Chemistry Practical-II
26	16PCH4PJ01	Project

16PCH1MC01 ORGANIC REACTION MECHANISMS AND STEREOCHEMISTRY

SEMESTER	**I**	**CREDITS**	**4**
CATEGORY	**MC(T)**	**NO.OF HOURS/ WEEK**	**6**

Objectives

1. To understand the path, feasibility and mechanism of a reaction.
2. To understand the techniques involved in the determination of mechanism of reactions and to propose methods to determine the mechanism of reaction.
3 To understand the concept of stereochemistry and reaction mechanism.
4 To suggest synthetic route for simple organic compounds based on stereochemistry.

Unit-1: Mechanisms and Methods (1+15+1 h)

1.1 Types of mechanism, reagents and reactions. Electronic effects, Thermodynamic and kinetic requirements of reactions; Hammond postulate; microscopic reversibility. Potential energy diagrams, transition states and intermediates.

1.2 Methods of determining mechanism: Non-kinetic methods- Product analysis; Determination of the presence of intermediates-isolation, detection, trapping; cross-over experiments isotopic labeling and isotope effects; stereo chemical evidence. Kinetic methods - relation of rate with the mechanism of reaction.

1.3 Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes. Effect of structure on reactivity. The Hammett and Taft equation and linear free energy relationship, partial rate factor, substituent and reaction constants.

Unit-2: Rearrangement Reactions (1+15+1 h)

2.1 Types of rearrangements: Nucleophilic, free radical and electrophilic reactions.

2.2 Mechanisms: Nature of migration; migratory ability and memory effects, Wagner-Meerwin reactions, rearrangement of 1,2-Glycols, Demjanov,Wolff, Benzil-benzilic acid, Favorskii, Hoffmann,Curtius, Lossen, Schmidt, Beckmann, Neber, Baeyer-Villiger, Stevens, Claisen, Fries and photo Fries, Benzidine, Cope and oxy-cope, Dakin rearrangements, boron-carbon migration, non-1,2-rearrangements, Fischer-indole synthesis, Arndt-Eistert synthesis.

Unit-3: Oxidation and Reduction Reactions (1+15+1 h)

3.1 Mechanisms: direct electron transfer, hydride transfer, hydrogen transfer, displacement, addition-elimination and formation of ester intermediates, Oxidative and reductive coupling reactions.

3.2 Oxidation Reactions: Dehydrogenation by quinones, selenium dioxides, ferricyanide, manganese dioxide, permanganate, mercuric acetate leadtetraacetate, and OsO_4 oxidation of saturated hydrocarbons, alkyl groups, alcohols, halides and amines; Reactions involving cleavage of C-C bonds: cleavage of double bonds; oxidative decarboxylation, allylicoxidation, Oxidation by chromium trioxide-pyridine, Dimethylsulphoxide-dicyclohexylcarbodiimide (DMSO-DCCD).

3.3 Reduction Reactions: Replacement of oxygen by hydrogen - Wolff Kishner and Clemmenson and Rosenmund reductions with mechanism; Electrochemical and photochemical reduction, Trialkyl and triphenyltin hydrides, McFadyen-Stevens reduction, Homogeneous hydrogenation, Reduction by metal hydrides and alkoxides with stereochemistry, Hydroboration with cyclic systems, Removal of Oxygen from substrate; Reduction with cleavage; MPV, Bouveault-Blanc reduction, reduction involving anionic attack.

Unit-4: Stereochemistry-I (1+15+1 h)

4.1 Introduction to molecular symmetry and chirality – axis, plane, center, alternating axis of symmetry. Optical isomerism due to asymmetric and dissymmetric molecules with C, N, S based chiral centers. Optical purity, prochirality, enantiotopic and diastereotopic atoms, groups and faces, chirality due to helical shape, methods of determining the configuration.

4.2 Racemic modifications: Racemisation by thermal, anion, cation, reversible formation; epimerisation, mutarotation.

4.3 Cram's and Prelog's rules; D, L, R, S-notations; proR, proS, side phase and re phase Cahn-Ingold-Prelog rules, absolute and relative configurations; Configurations of allenes, spiranes, biphenyls, cyclooctene, helicene,binaphthyls, ansa and cyclophanic compounds, exo-cyclic alkylidene-cycloalkanes, and exo-cyclic alkylidenecycloalkanes. Topicity and prostereoisomerism – NMR distinction of enantiotopic/diastereotopiccompounds.

4.4 Criteria for optical purity; Resolution of racemic modifications; asymmetric transformations; asymmetric synthesis; destruction. Optical purity calculations.

4.5 Geometrical isomerism: E, Z notations, geometrical isomerism in C=C, cyclic systems and oximes.

Unit-5: Stereochemistry-II (1+20+1 h)

5.1 Conformation and reactivity of acyclic systems; intramolecular rearrangement; neighbouring group participation; chemical consequence of conformational equilibrium - Curtin-Hammett principle.

5.2 Stability of five and six-membered rings; mono and disubstitutedcyclohexanes; conformation and reactivity in cyclohexane systems.

5.3 Fused and bridged rings; bicyclic and poly cyclic systems; decalins and Brett's rule.

5.4 Optical rotation and optical rotatory dispersion; conformational asymmetry, ORD curves; octant rule; configuration and conformation; Cotton effect; axial haloketone rule; Determination of configuration.

5.5 Stereoselective and stereospecific synthesis.

Text books

1. J. March and M. Smith, *Advanced Organic Chemistry*, 5th ed., John-Wiley and Sons. 2001.
2. E. S. Gould, *Mechanism and Structure in Organic Chemistry*, Holt, Rinehart and Winston Inc., 1959.
3. P. S. Kalsi, *Stereochemistry of carbon compounds*, 8th edn, New Age International Publishers, 2015.
4. P. Y.Bruice, *Organic Chemistry*, 7th edn.,Prentice Hall, 2013.
5. R. T. Morrison, R. N. Boyd, S. K. Bhattacharjee*Organic Chemistry*, 7th edn., Pearson Education, 2010.
6. D. Nasipuri, *Stereochemistry of Organic Compounds, 2nd ed,*, New Age Publishers, 2005.
7. S. M. Mukherji and S. P. Singh, *Reaction Mechanism in Organic Chemistry*, 3rd ed., Macmillan India Ltd. 1984.

References

1. F.A. Carey and R.J. Sundberg, *Advanced Organic Chemistry Part-A and B,* 5th Edn, Kluwer Academic / Plenum Publishers. 2007.
2. D. G. Morris,*Stereochemistry*, RSC Tutorial Chemistry Text 1, 2001
3. N.S. Isaacs, *Physical Organic Chemistry*, ELBS. Longman, UK, 1987.
4. E. L. Eliel, *Stereochemistry of Carbon Compounds*, Tata-McGraw Hill, 2000.
5. I. L. Finar, *Organic Chemistry. Vol-2*, 5th ed., Pearson Education Asia, 1975.
6. I. L. Finar, *Organic chemistry, Vol-1,* 6th ed., Pearson Education Asia, 2004.

7. T. H. Lowry K. S. Richardson, Harper and Row*Mechanism and theory in organic chemistry*, 2nd edn., New York, 1981.
8. S. H. Pine, *Organic Chemistry, 5th ed.*, McGraw Hill International Ed., 1987.
9. L. F. Fieser and M. Fieser, *Organic Chemistry*, Asia Publishing House, Bombay, 2000.
10. G. C. Barret, *Elucidation of Organic structures by Physical and Chemical Methods Part I* (Eds) K.W. Bentley and G.W.Rirty John Wiley, 1972, Chapter VIII.

16PCH1MC02 CONCEPTS IN INORGANIC CHEMISTRY

SEMESTER	**I**	**CREDITS**	**4**
CATEGORY	**MC(T)**	**NO.OF HOURS/ WEEK**	**5**

Objectives

1. To understand the different kinds of chemical forces in molecules.
2. To identify the nature of chemical bond in a given inorganic compound.
3. To predict the nature and topology of inorganic compounds.
4. To know the existence of compounds through weak chemical forces.
5. To identify relevant inorganic compounds for specific applications.

Unit-1: Atomic Structure and Periodic Table

1.1 Periodicity, Structure of atom, Bohr's theory.

1.2 Modern views on atomic structure: Wave mechanical description of electron and orbitals- radial density functions and orbital energies, angular functions and orbital shapes.

1.3 *Slater orbitals and their uses*: computation of effective nuclear charge and radii of atoms and ions.

Unit-2: Ionic Compounds

2.1 Packing of ions in crystals and crystal structures-*ccp*, *hcp*, *bcc*, and *fcc*.

2.2 *Radius ratio and structure of ionic lattices*: Geometrical method of computing radius ratio, radius ratio and coordination number, stoichiometry and crystal structures. Madelung constant.

2.3 *Lattice energy*: derivation of Born-Lande equation, modified Born-Lande equation, factors affecting lattice energy. Layer lattices, applications.

2.4 *Born-Haber cycle*: Thermochemical calculations, radii of nonspherical ions, solubility and thermal properties of ionic compounds as a function of U_o and ΔH_f.

2.5 *Polarization in ionic compounds*: covalency and Fajan's rules, effects of polarization.

Unit-3: Covalent Bond

3.1 *Molecular topologies*: shared and lone pairs and Lewis structures, isoelectronic and isolobel relationships, hybridization and geometry, VSEPR model, and Bent's rule.

3.2 *Molecular Orbital Theory*: Symmetry of molecular orbitals formed from atomic orbital overlap, Extended Huckel theory of Hartree-Fock approximation (SCF), LCAO-MO model, TASO, LUMO, and HOMO concepts in bonding.

3.3 MO energy level diagrams of homo- and heterodiatomic molecules (CO, NO, and HCl).

3.4 *Bonding in metals*: packing of atoms in metals, band theory of metals and metallic properties, insulators, and semiconductors.

Unit-4: Weak Chemical Forces

4.1 *van der Waals forces*: Inclusion compounds-layer, channel, and cage structures (gas hydrates and clathrates).

4.2 *Hydrogen bonding*: associated molecules, and molecular self-assembly.

4.3 Supramolecular architectures formed by weak chemical forces.

Unit-5: Acid-base Theory and Solvent Systems

5.1 *Acid-Base theories*: Bronsted-Lowry, Lux-Flood, Usanovich, Lewis, and solvent system. definitions, measures of acid-base strength, acid-base interactions, hard and soft acid and bases, classification, levelling effect, symbiosis, proton sponges.

5.2 *Nonaqueous solvents*: Classification-protonic and aprotic solvents, super acids, molten salts as solvents. ionic liquids and their use in synthesis.

5.3 Hard soft acid base principle: theoretical basis of hardness, class A and B.

Text Books

1. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*; 6th ed.; Wiley Interscience: New York, 1988.
2. K. F. Purcell and J. C. Kotz, *Inorganic Chemistry*; Saunders: Philadelphia, 1976.
3. J. E. Huheey, E. A. Keiter and R. L. Keiter, *Inorganic Chemistry*; 4th ed.; Harper and Row: NewYork, 1983.
4. B. E. Douglas, D. H. McDaniel and J. J. Alexander, *Concepts and Models of Inorganic Chemistry*; 3rd ed.;John Wiley & Sons, 1994.

References

1. T. Moeller, *Inorganic Chemistry, A Modern Introduction*; John Wiley: New York, 1982.
2. D. F. Shriver, P. W. Atkins and C.H. Langford; *Inorganic Chemistry*; 3rd ed.; Oxford University Press: London, 2001.
3. G. H. Stout and L. H. Jenson, *X-Ray Structure Determination*; 2nd ed.; John Wiley & Sons: New York, 1989.

4. A. R. West, *Solid State Chemistry and its Applications*; John Wiley & Sons: New York, 1989.
5. G. Rhodes, *Crystallography Made crystal Clear*; Academic Press, Inc.: New York, 1993.
6. C. Hammond, *The Basics of Crystallography and Diffraction*; Oxford University Press; 1997.
7. L. Smart and E. Moore, *Solid State Chemistry, An Introduction*; 2^{nd} edn.; Nelson Thornes Ltd., Cheltenham, 1996.

16PCH1MC03 QUANTUM CHEMISTRY AND GROUP THEORY

SEMESTER	**I**	**CREDITS**	**4**
CATEGORY	**MC(T)**	**NO.OF HOURS/ WEEK**	**6**

Objectives

1. To understand the physical and mathematical aspects of quantum mechanics and familiarize the mathematics required for solving quantum mechanical problems.
2. To understand the quantum mechanical approach to atomic and molecular electronic structure.
3. To understand the importance of symmetry and its applications.

Unit-1: Mathematics for Quantum Mechanics and Postulates of Quantum Mechanics

(1+12+1 h)

1.1 Mathematical concepts: Coordinate systems: Cartesian, spherical polar, cylindrical and elliptical coordinate systems. Functions: Real, complex, odd, even, orthogonal, normalized and eigen functions, eigen values and orthonormal set. Differential equations: Order and degree. Solutions to typical differential equations. Operators: linear, angular, differential, Hermitian and Hamiltonian operators.

1.2 Introduction to Quantum Mechanics: Failure of classical mechanics: Black body radiation, photo electric effect, hydrogen atomic spectrum and Compton effect. The need for quantum mechanics. Postulates of Quantum Mechanics and Schrodinger wave equation.

Unit-2: Some Quantum mechanical models and their applications (1+14+1 h)

2.1 Particle in a box (1D and 3D). Degeneracy and its application to linear conjugated molecular systems, free particle. Bohr's correspondence principle. Quantum mechanical tunneling: Tunneling in chemical reactions (electron transfer), inversion of ammonia, proton transfer reactions.

2.2 Rigid Rotor: Wave equation and solution. Calculation of rotational constants and bond length of diatomic molecules.

2.3 Harmonic Oscillator: Wave equation and solution. Anharmonicity. Force constant and its significance

Unit 3: Application of Quantum Mechanics to Hydrogen and poly electron atoms (1+21+1 h)

3.1 Hydrogen atom and hydrogen like ions: Hamiltonian - wave equation and solution to hydrogen and hydrogen like systems. Radial and angular functions. Quantum numbers n, l, m and s and their importance. Radial distribution functions and their representation.

3.2 Approximation Methods: Variation method-Trial wave functions. Variation integral and its application to particle in a 1D box. Perturbation method and its application. Hartree-Fockself-consistent field method.

3.3 Quantum mechanical treatment of angular momentum - Simultaneous measurement. Commutators: $[x, p_x]$,$[x, p_x^2]$,[Lx, Ly] and $[Lx^2, Lx]$ and their significance.

3.4 Helium atom: Electron spin, Pauli Exclusion Principle and Slater determinant. Derivation of atomic term symbols.

Unit4: Molecular Quantum Mechanics and Chemical bonding (1+13+1 h)

4.1 Hydrogen molecule: Molecular orbital theory and Heitler-London (VB) treatment. Energylevel diagram.

4.2 Hydrogen molecular ion: Use of linear variation function and LCAO methods.

4.3 Electronic structure of conjugated systems: Huckel method applied to ethylene, allyl systems, butadiene and benzene.

Unit 5: Group theory and applications (1+20+1 h)

5.1 Group and subgroup. Symmetry elements and operations. Classification of molecules into non axial, axialand dihedral point groups - C_{nv}, C_{nh}, D_n, D_{nh}, D_{nd}, $T_d$and O_h.

5.2 Matrix representations of symmetry operations. Reducible and irreducible representations. Classes of operations.

5.3 The Great orthogonality theorem: Reduction formula, construction of character table for C_{2v}, $C_{2h}$and C_{3v} point groups.

5.4 Application of group theory to molecular vibrations, electronic spectra of formaldehyde and ethylene, chemical Bonding.

Text books

1. R.K. Prasad. *Quantum Chemistry through problems and Solutions*, New Age International Publishers, New Delhi.1997.
2. A. Vincent- *Molecular Symmetry and Group Theory*. *A Programmed Introduction toChemical Applications*.John and Willy & Sons Ltd. 1977.
3. D. A. McQuarie, *Quantum Chemistry*. Viva Books PW. Ltd., New Delhi. 2003.
4. T.Engel and R.Philip,*Quantum Chemistry And Spectroscopy*,5^{th} edition, Pearson, NewDelhi,2006.

5. F. A. Cotton, *Chemical Applications of Group Theory*. 2nd edition, John Wiley & Sons, 1971.
6. K. V. Raman, *Group Theory and its Applications to Chemistry*, Tata McGraw-Hill, NewDelhi, 1990.

References

1. N.Levine, *Quantum Chemistry*, 4th edition, Allyn& Bacon Inc., 1983.
2. D.A. McQuaric and J. D. Simon. *Physical Chemistry, A Molecular Approach*, Viva Books Pvt. Ltd., New Delhi. 1998.
3. R. P. Rastogi and V. K. Srivastava. *An Introduction to Quantum Mechanics of ChemicalSystems*.Oxford& IBH Publishing Co., New Delhi 1986,
4. R.L. Flurry. Jr. *Symmetry Group Theory and Chemical applications*, PrenticeHall.Inc. 1980.
5. J. M. Hollas, *Symmetry in Molecules*, Chapman and Hall, London, 1972.
6. H. Eyring, J. Walter and E. Kimball, *Quantum Chemistry*, Wiley International edition, JohnWiley, London, 1989.
7. W. J Moore, *Physical Chemistry*, Longman, 5th edition, London, 1974.
8. G. W. Castellan, *Physical Chemistry*, Addison-Wesley, 4th edition, London, 1996.

16PCH1MC04 ANALYTICAL CHEMISTRY

SEMESTER	**I**	**CREDITS**	**4**
CATEGORY	**MC(T)**	**NO.OF HOURS/ WEEK**	**5**

Objectives

1. To learn the basic analytical methods and to have a knowledge of chemistry involved in chemical analysis.
2. To know the principle and instrumentation of different analytical techniques.

Unit 1: Data Analysis (1+10+1 h)

1.1 Errors: Precision and accuracy, Classification of errors, methods of minimization and elimination of errors.

1.2 Statistical methods: Treatment of random errors, reliability of results, rounding up of results from chemical computation, confidence interval, Normal error curve and its importance. Comparison of results : students t-test, F-test and linear regression for deriving calibration plots.

Unit 2: Chromatography (1+13+1 h)

2.1 Principles of thin layer, paper and column chromatographic techniques.

2.2 Gas chromatography: carrier gas, columns, detectors-hot-wire detector, flame ionization detector, photo ionization detector and ECD. Determination of C,H,N and S.

2.3 HPLC: Column, solvent delivery system, sample injections, Detectors. Advantages of HPLC. Applications of HPLC in the separation of cations. Principles of preparative and analytical HPLC.

2.4 Electrophoresis and capillary electrophoresis – principle, instrumentation and applications.

Unit 3: Titrimetric Methods of Analysis (1+13+1 h)

2.1 Difference between titrimetic and volumetric analysis, Principle and reactions involved in acid-base, redox, complexometric and precipitation titrations, Different methods of expressing concentration terms, calculations involving stoichiometry- acid base and redox systems.

2.2 Acid-base titrations in non-aqueous solvents: Principle, properties – acidic and basic properties, auto-protolysis constant of solvents, dielectric constant and its effect on solvent behaviour. Detection of equivalence point – titrations in ethylene diamine, glacial acetic acid, methanol and ethanol.

2.3 Hydrolysis of salts – hydrolysis of a salt of a strong base / weak acid, weak base / strong acid and weak acid / weak base.

Unit 4: Thermal and Electroanalytical Methods (1+16+1 h)

4.1 Thermogravimetry: Principle, factors affecting thermogram, instrumentation and thermal decomposition of $CaC_2O_4.H_2O$ and $CuSO_4.5H_2O$. Differential techniques: Instrumentation, experimental and instrumental factors of DTA. Thermal behaviour of $CuSO_4.5H_2O$ by DTG. Principle and determination of purity of pharmaceuticals, phase transition studies by DSC.

4.2 Electrogravimetry: Principle, instrumentation, deposition and separation. Electrolysis at constant current and estimation of copper.

4.3 Coulometry: controlled potential coulometry, Principle and separation of nickel and cobalt, coulometric titration, instrumentation - Estimation of Sb(III).

4.4 Potentiometry: Potentiometric titration, equivalence point potential for (i) Fe^{2+}/ Fe^{3+}-Ce^{3+}/Ce^{4+} (ii) Fe^{2+}/ Fe^{3+}- MnO_4^-, H^+/Mn^{2+} systems. Determination of concentration of the species at the equivalence point. Ion selective electrodes, coated/modified electrodes, Biochemical electrodes. Solid state ion selective detectors.

Unit-5: Spectrometry (1+13+1 h)

5.1 Spectrophotometry: Beer-Lambert's law, spectrophotometric titrations, determination of Fe(III) with EDTA and determination of Fe(III) in the presence of aluminium.

5.2 Atomic Absorption Spectroscopy: Principle, instrumentation - Burner, furnace, resonance line source, detectors. Spectral and chemical interferences, determination of alkali metals in blood serum, Determination of lead in petrol. Principle of Inductively coupled plasma (ICP) spectrometry.

5.3 Flame emission spectrometry: Principle, instrumentation and interferences, determination of alkali metals, Determination of iron in non-ferrous alloys.

5.4 Turbidimetry and nephlometry: Principle, instrumentation - determination of sulphate and phosphate.

5.5 Fluorimetry: Principle, relationship between excitation spectra and fluorescence spectra, factors affecting fluorescence emission, determination of quinine in tonic water and determination of codeine and morphine in a mixture.

Books for study:

1. Douglas A. Skoog, Donald M. West and F. James Holler, *Fundamentals of analytical Chemistry*, 9^{th} Ed., Harcourt Asia Pvt. Ltd., 2013.
2. R. A. Day, Jr. and A.L. Underwood, *Analytical Chemistry*, Prentice-Hall of India, 2001.
3. H. Kaur, *Instrumental methods of chemical analysis*, Pragati Prakashan, 2003.
4. G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denney, *Vogel's Textbook of Quantitative Chemical Analysis*, Longman Scientific and Technical, 1989.

Books for reference:

1. D. A. Skoog, D. M. West and F. J. Holler, *Analytical Chemistry an Introduction*, Saunders College Publishers, 1990.
2. J. Mendham, R. C. Denney, J. D. Barnes and M. Thomas, *Vogel's Text book of Quantitative Chemical Analysis*, Pearson Education Pvt. Ltd., 2004.
3. J. G. Dick, *Analytical Chemistry*, Sir George Williams University, McGraw-Hill Book Company, New York, 1973.

4. H. H. Willard, L. L. Merritt, J. A. Dean and F. A. Seattle, *Instrumental methods of analysis*,5th Ed., Harcourt Asia Pvt. Ltd., India, 2001.
5. E. Heftmann, *Chromatography: Fundamentals and applications of chromatography and related differential migration methods - Part A: Fundamentals and techniques*, Elsevier, 2004.
6. M. G. Gore, *Spectrophotometry and Spectrofluorimetry: A Practical Approach*, Oxford University Press, 2000.

16PCH1MC05 ORGANIC LABORATORY TECHNIQUES-I

SEMESTER	**I**	**CREDITS**	**2**
CATEGORY	**MC(L)**	**NO.OF HOURS/ WEEK**	**4**

Objectives

To develop analytical skill in

(i) Separation of organic mixture
(ii) Organic qualitative analysis
(iii) Organic preparations involving two stages.

1. **Separation and analysis**: Two component mixtures.
2. **Preparations**: Two stage processes involving nitration, halogenation, diazotization, rearrangement, hydrolysis, reduction, alkylation and oxidation. Two stage preparations

a) *p*-Bromoacetanilide from Aniline (Acetylation-bromination)
b) *p*-Nitroaniline from Acetanilide (nitration-hydrolysis)
c) 1,3,5-Tribromobenzene from Aniline (bromination-deamination)
d) Acetyl salicyclic acid from Methyl salicylate (Esterification-Hydrolysis)
e) Benzilic acid from Benzoin (oxidation - rearrangement)
f) *m*-Nitroaniline from Nitrobenzene (Nitration-Reduction)

Text books

1. N. S. Gnanapragasam and G. Ramamurthy, *Organic Chemistry – Labmanual*, S. Viswanathan Co. Pvt. Ltd, 1998.
2. J. N. Gurtu and R. Kapoor, *Advanced Experimental Chemistry*, S. Chand and Co., 1987

Reference

1. Vogel's *Text book of Practical Organic Chemistry*, 5th Ed, ELBS/Longman, England, 1984.

16PCH1MC06 INORGANIC QUANTITATIVE ANALYSIS AND PREPARATIONS

SEMESTER	**I**	**CREDITS**	**2**
CATEGORY	**MC(L)**	**NO.OF HOURS/ WEEK**	**4**

Objectives

1. To impart the skill in estimation of metal ions by colorimetric and complexometric methods.
2. To identify the methodology to estimate a metal ion in the presence of another metal ion.
3. To impart the skill in preparations of metal complexes.

1. Colorimetry (visual**)**

1.1 Estimation of iron.
1.2 Estimation of nickel.

2. Complexometric Titration

2.1 Estimation of zinc, nickel, magnesium, and calcium.
2.2 Estimation of mixture of metal ions-pH control, masking and demasking agents.
2.3 Determination of calcium and lead in a mixture (pH control).
2.4 Determination of manganese in the presence of iron.
2.5 Determination of nickel in the presence of iron.

3. Gravimetry and Titrimetry

3.1 Determination of nickel by gravimetry and copper by titrimetry in a mixture.
3.2 Determination of barium by gravimetry and calcium by complexometry in a mixture.

4. Preparations and estimation of one metal ion in one experiment

4.1 Potassium tris(oxalato)ferrate(III)
4.2 Hexaamminenickel(II) tetrafluoroborate
4.3 Potassium tetrachlorocuprate(II)
4.4 Tris(thiourea)(sulfato)zinc(II)

5. Determination of iron by colorimetry and calculation of percentage of Fe in $K_3[Fe(C_2O_4)_3]$.

Text books

1. G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denney, *Vogel's Textbook of Quantitative Chemical Analysis*; 5th ed., ELBS, 1989.
2. J. D. Woollins, *Inorganic Experiments*; VCH: Weinheim, 1994

References

3. G. Pass, and H. Sutcliffe, *Practical Inorganic Chemistry*; Chapman Hall, 1965.
4. W. G. Palmer, Experimental *Inorganic Chemistry*; Cambridge University Press, 1954.

16PCH2MC01 ORGANIC REACTION MECHANISM AND HETEROCYCLIC COMPOUNDS

SEMESTER	**II**	**CREDITS**	**4**
CATEGORY	**MC(T)**	**NO.OF HOURS/ WEEK**	**5**

Objectives

1. To understand the mechanism of organic chemical reactions.
2. To appreciate the concept of substitution, addition and elimination reactions and their reaction mechanisms.

3. To comprehend the importance of heterocyclic compounds.

Unit-1: Aromatic and Aliphatic Electrophilic Substitution (1+18+1 h)

1.1 Aromaticity:Aromaticity in benzenoid, non-benzenoid, heterocyclic compounds and annulenes; alternant and non-alternant hydrocarbons, Huckel's rule, energy level of π-molecular orbitals, antiaromaticity, homo-aromaticity, PMO approach. Bonds weaker than covalent, addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes; NMR as a tool for aromaticity - anti- and homo-aromatic systems.

1.2 Aromatic electrophilic substitution: Mechanism, orientation and reactivity - Quantitative treatment of reactivity in the substrates and reactivity of the electrophiles.

1.3 Reactions involving nitrogen electrophiles: nitration, nitrosation and diazoniumcoupling; Sulphur electrophiles: sulphonation; Halogen electrophiles: chlorination and bromination; Carbon electrophiles: Friedel-Crafts alkylation, acylation and arylation reactions.

1.4 Aliphatic substitution Mechanisms: SE2 and SEi, SE1; Substitution by double bond shifts; other mechanism: addition-elimination and cyclic mechanism.

1.5 Hydrogen as electrophile: (a) Hydrogen exchange; hydro dehydrogenation; ketoenoltautomerism. b) Halogen electrophiles: Halogenation of aldehydes, ketones and carboxylic acids c) Nitrogen electrophiles: aliphatic diazonium coupling; direct formation of diazo compounds; direct amination; insertion by nitrenes. d) Sulphur electrophiles: sulphonation, sulphenylation. e) Carbon electrophiles: acylation; alkoxy carbonyl alkylation; alkylation; Stork-enamine reaction; insertion by carbene.

Unit-2: Aromatic and Aliphatic Nucleophilic Substitution (1+13+1 h)

2.1 Mechanisms: S_NAr, S_N1 and Benzyne mechanisms. - Reactivity, Effect of structure, leaving group and attacking nucleophile.

2.2 Reactions: Oxygen and Sulphur-nucleophiles, Bucherer and Rosenmund reactions, von Richter, Sommelet-Hauser and Smiles rearrangements. S_N1, ion pair, S_N2 mechanisms and evidences. Nucleophilic substitutions at an allylic carbon, aliphatic trigonal carbon and vinyl carbon.S_N1, S_N2, S_Ni, and S_E1 mechanism- Neighbouring group participation- Non classical carbocations. Reactivity: Effect of substrate, attacking nucleophile, leaving group and the medium - Swain-Scott, Grunwald-Winstein relationship - Ambident nucleophiles.

Unit-3: Elimination and Free Radical Reactions (1+13+1 h)

3.1 Mechanisms: E2, E1, and E1cB mechanisms. Syn eliminations - E1-E2-E1cB spectrum. Orientation of the double bond: Hoffmann and Saytzeff rules

Reactivity: Effect of substrate, attacking bases, leaving group and medium. Mechanisms and orientation in pyrolyticeliminations. Elimination reactions: Stereochemistry of eliminations in acyclic and cyclic systems, orientation in eliminations - Saytzeff and Hoffman elimination, propolitic elimination.

3.2 Long lived and short lived radicals – Production of radicals by thermal and photochemical reactions, Detection and stability of radicals, characteristics of free radical reactions and free radical, reactions of radicals; polymerization, addition, halogenations, aromatic substitutions, rearrangements. Reactivity: Reactivity on aliphatic, aromatic substrates, reactivity in the attacking radical, effect of solvent.

Unit-4: Addition to Carbon Multiple Bonds (1+10+1 h)

4.1 Mechanisms: (a) Addition to carbon-carbon multiple bonds- Addition reactions involving electrophiles, nucleophiles, free radicals, carbenes and cyclic mechanisms-Orientation and reactivity, hydrogenation of double and triple bonds, hydroboration, Birch reduction, Michael reaction, addition of oxygen and Nitrogen; (b) Addition to carbon-hetero atom multiple bonds: Mannich reaction, LAH reduction of Carbonyl compounds, acids, esters, nitrites, addition of Grignard reagents, Reformatsky reaction, Tollen's reaction, Wittig reaction, Prins reaction.

4.2 Stereochemical aspects of addition reactions. Addition to Carbon-Hetero atom Multiplebonds**:** Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds. Mechanism of condensation reactions involving enolates – Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.

Unit-5: Heterocyclic Chemistry (1+11+1 h)

5.1 Nomenclature, reactivity, aromaticity, spectral properties.

5.2 Synthesis and reactions of indole, isoindole, oxazole, imidazole, thiazole, pyridine, pyrimidine, pyridazine, pyrazine, chromans, chromons, coumarins, carbazoles, uracil, uric acid and xanthines.

5.3 Oxygen Heterocyclic Compounds: Classification, color reactions of various classes of flavonoids – chemistry and synthesis of flavones (luteolin), isoflavones (daidzein), flavonols (kaempferol) and anthocyanidins (cyanidin).

Text books

1. J. March and M Smith, *Advanced Organic Chemistry*, 5thed., John-Wiley and sons, 2001.
2. I. L. Finar, *Organic Chemistry* Vol-2, 5thedn., Pearson Education Asia, 1975.
3. I. L. Finar, *Organic Chemistry* Vol-1, 6thedn., Pearson Education Asia, 2004.
4. F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry*, Part A and B, 5thed., Kluwer Academic/Plenum Publishers, 2008.
5. S.M.Mukherji and S.P.Singh, *Reaction Mechanism in Organic Chemistry*, 3rd ed., Macmillan India Ltd. 1984.

References

1. S. H. Pine, *Organic Chemistry*, 5thedn, McGraw Hill International Editionn, 1987.
2. L. F. Fieser and M. Fieser, *Organic Chemistry*, Asia Publishing House, Bombay, 2000.
3. E.S. Gould, *Mechanism and Structure in Organic Chemistry*, Holt, Rinehart and Winston Inc., 1959.
4. T. L. Gilchrist, *Heterocyclic Chemistry*, Longman Press, 1989.
5. J. A. Joule and K. Mills, *Heterocyclic Chemistry*, 4thed., John-Wiley, 2010.
6. K. S. Richardson and T. H. Lowry, *Mechanisms and Theory in Organic Chemistry* by 3rd ed., Joanna Cotler Books, 1981.
7. T. H. Lowry K. S. Richardson, Harper and Row, *Mechanism and theory in organic chemistry*, 2nd, New York, 1981.
8. S. H. Pine, *Organic Chemistry, 5thed.*, McGraw Hill International Ed., 1987.
9. L. F. Fieser and M. Fieser, *Organic Chemistry*, Asia Publishing House, Bombay, 2000.

16PCH2MC02
COORDINATION CHEMISTRY

SEMESTER	**II**	**CREDITS**	**4**
CATEGORY	**MC(T)**	**NO.OF HOURS/ WEEK**	**5**

Objectives

1. To know the nature of metal-ligand bonding in coordination compounds and bonding parameters.
2. To know the chemical and photochemical behaviour of coordination compounds.
3. To know the mechanisms of reactions of coordination compounds.
4. To understand the importance of coordination compounds in the emerging field of supramolecular chemistry and nanotechnology.
5. To know the application of coordination compounds in catalysis and biology.

Unit-1: Theories of Coordination Compounds

1.1 Structural features of complexes of coordination numbers 2 to 6 and higher coordination numbers.

1.2 Crystal Field Theory: inadequacy of valence bond theory, crystal field splitting in T_d and O_h fields, high spin vs low spin complexes, spin crossover. Computation of CFSE in tetrahedral geometry and LS and HS octahedral geometries, factors which determine 10Dq values, spectrochemical series. Evidences of crystal field splitting.

1.3 Jahn-Teller theorem: Jahn-Teller effect-consequences, static and dynamic Jahn-Teller effect. Tetragonal distortions from O_h symmetry and crystal field splitting in tetragonally distorted octahedral and square planar geometries.

1.4 Molecular Orbital Theory: Evidences of metal-ligand covalency, TASO-MO concepts of O_h and T_d complexes, MO energy level diagrams of σ- and π-

bonding in O_h complexes, nature of metal-ligand π-bonds, evidences for π-back bonding, spectrochemical series, and π- acceptor series, evidences for back bonding from vibrational spectroscopies.

1.5 Angular Overlap Model: Principles, quantification of metal-ligand orbital interactions (e_σ- and e_π-parameters), angular overlap and geometry, angular scaling factors for e_σ- and e_π- parameters, computation of Δ_o and Δ_τ and their relationship.

Unit-2: Electronic Structure and Geometry of Coordination Compounds

2.1 Molecular magnetism: diamagnetic and paramagnetic susceptibilities, temperature dependent paramagnetism, the Curie law, ferromagnetic and antiferromagnetic interactions. Methods of determining magnetic susceptibility: Gouy and Faraday balances, vibrating sample magnetometer (VSM) and SQUID. Van Vleck equation and magnetic moments of free metal ions.

2.2 IR spectroscopy: differentiation of linkage isomers-cyano- and isocyano-, nitro- and nitrito-, thiocyanato- and isothiocyanato complexes, IR spectra of terminal and bridging carbonyls.

2.3 Electronic absorption spectroscopy: derivation of term symbols, electronic states and spectra of O_h and T_d complexes of d^n metal ions, Orgel and Tanabe-Sugano diagrams.

Unit-3: Organometallic Compounds and Reaction Mechanisms

3.1 Classification of reaction types: reactions involving (a) change in the composition and (b) change in the position of ligand in the coordination sphere, (c) electron transfer reactions.

3.2 *Trans*-effect and synthesis of square planar complexes; mechanism of replacement of coordinated water in O_h

complexes: D, A, I_a and I_d mechanisms; hydrolysis of O_h complexes.

3.3 Electron transfer reactions: mechanisms of inner- and outer-sphere and long range electron transfers.

3.4 Nomenclature of chiral complexes, study of absolute configurations of chiral complexes-ORD and CD, the hapto nomenclature in organometallic chemistry.

3.5 Structure and bonding in metal alkenes, metal-alkynes, and organometallic compounds of cyclic- and open chain π-donors, metallocenes, metal-aryls, double- and triple decker sandwich complexes.

3.6 Catalysis involving organometallic compounds: alkene isomerization and metathesis; Ziegler-Natta catalyst and alkene polymerization; Wilkinson catalyst and alkene hydrogenation; carbonylation, hydroformylation, hydrocarboxylation, Fischer-Tropsch synthesis, Wacker process.

Unit-4: Supramolecular Chemistry and Photochemistry

4.1 Crystal field and charge transfer (MLCT, CTTM) photochemistry: photosubstitution and photoisomerization reactions.

4.2 Molecular recognition: molecular receptors, recognition of neutral molecules anions and cations.

4.3 Macrocyclic complexes. Supramolecular assemblies and architectures: nature of supramolecular interactions, supramolecular assemblies formed by templates and self-assembly.

Unit-5: Bioinorganic Chemistry

5.1 Metalloproteins and enzymes-general introduction and properties.

5.2 Heme proteins: haemoglobin and myoglobin-structure, mechanism of oxygen transport; cytochromes-biological roles and structural features.

5.3 Copper proteins: structure and functions of type-I, type-II and type-III.

5.4 Photosynthesis: chlorophyll, photosystem-I and photosystem-II, photosynthetic reaction center and *Z*-scheme.

5.5 Enzymes: superoxide dismutase, carboxy peptidase *A*-structure and functions.

Text Books

1 J. E. Huheey, E. A. Keiter, R. L. Keiter, *Inorganic Chemistry*, 4th ed.; Harper and Row: New York, 1983.

2 F. A. Cotton, G. Wilkinson.; C. A. Murillo; M. Bochmann, *Advanced Inorganic Chemistry*, 6th ed.; Wiley Inter-science: New York, 1988.

3 K. F. Purcell, J. C. Kotz, *Inorganic Chemistry*; Saunders: Philadelphia, 1976.

4 R. S. Drago, *PhysicaI Methods in Chemistry*; Saunders: Philadelphia, 1977.

5. K. K. Rohatgi Mukherjee, *Fundamentals of photochemistry (Revised edition)*, Wiley Eastern Ltd., 1996.

References

1. K. Nakamoto, *Infrared and Raman Spectra of Inorganic and coordination Compounds*, Part B: 5th ed.; John Wiley& Sons Inc.: New York, 1997.
2. A. B. P. Lever, *Inorganic Electronic Spectroscopy*, 2nd ed.; Elsevier: Amsterdam, 1984.
3. M. L. Tobe and J. Burgess, *Inorganic Reaction Mechanisms*; Longman: New York, 1999.
4. J. A. Weil, J. R. Bolton and J. E. Wertz, *Electron Paramagnetic Resonance*; Wiley Interscience: 1994.
5. O. Kahn, *Molecular Magnetism*, VCH: Weinheim, 1993.
6. J. W. Steed and J. L. Atwood, *Supramolecular Chemistry*, John Wiley & Sons Ltd.: New York, 2000.
7. J. M. Lehn, *Supramolecular Chemistry, Concepts and Prespectives*, VCH: Weinheim, 1995.
8. S. J. Lippard, and J. M. Berg, *Principles of Bioinorganic Chemistry*, University Science Books, New York, 1994.

16PCH2MC03 MOLECULAR SPECTROSCOPY

SEMESTER	**II**	**CREDITS**	**5**
CATEGORY	**MC(T)**	**NO.OF HOURS/ WEEK**	**6**

Objectives

1. To understand the quantization of energy and interaction of electromagnetic radiation with matter.
2. To understand the fundamentals of different branches of spectroscopy.
3. To elucidate the structures of molecules using different spectral techniques.

Unit 1: Rotational and Vibrational Spectroscopy

(1+23+1 h)

1.1 Diatomic molecules as rigid rotors - intensity of spectral lines, selection rules, effect of isotopic substitution. Diatomic molecules as non-rigid rotors -rotational spectra of linear and symmetric top polyatomic molecules.

1.2 Vibrating diatomic molecule - energy of diatomic molecules, simple harmonic oscillator –energy levels, transitions, selection rules. Anharmomic oscillator - energy levels, selection rules. Diatomic vibrating rotator - P, Q, R branches.

1.3 Vibrations of polyatomic molecules -Symmetry and fundamental vibrations, overtones, combination, difference bands. Influence of rotations on the spectra of polyatomic molecules - parallel and perpendicular vibrations in linear and symmetric top molecules.

1.4 Interpretation of IR spectra of organic and inorganic compounds - Frequencies of various functional groups containing oxygen, nitrogen and hydrocarbons. Factors affecting the fundamental vibrational frequencies. Linkage, geometrical isomers, coordinated and lattice water. NO_2, CO_3, ClO_4^-, and SO_4^{2-}.

1.5 Raman Effect -Rayleigh and Raman scattering, Stokes and anti-Stokes radiation, molecular polarizability, selection rules.

1.6 Raman spectra : Rotational Raman spectra - linear molecules, symmetric top and sphericaltop molecules. Vibrational Raman spectra - symmetry and Raman active vibrations, rule of mutual exclusion. Rotational fine structure. Structure determination from Raman and Infrared.

Unit 2: Electronic spectroscopy (1+ 13+1h)

2.1 Electronic spectra of diatomic molecules : Born-Oppenheimer approximation, Franck Condon Principle, selection rules, intensity of electronic transition, types of electronic transitions. Factors affecting the electronic transitions.

2.2 Characterization of organic compounds : application of Woodward-Fieser rules to conjugated dienes, α, β - unsaturated carbonyl compounds, benzene and its substituted derivatives, polycyclic aromatic hydrocarbons, polyenes, poly-ynes, and heterocyclic compounds.

2.3 Charge transfer transitions : Intensity, electronic spectra of charge transfer complexes of organic compounds, charge transfer transitions in inorganic and coordination compounds.

Unit 3: Mass spectroscopy (1+10+1h)

3.1 Determination of molecular formula - molecular ion, nitrogen rule, isotope peaks, metastable ions, Mc Lafferty rearrangement, Retro Diels Alder reaction.

3.2 Fragmentation - Basic fragmentation types and rules, Fragmentation patterns of hydrocarbons, oxygen and nitrogen containing organic compounds and carbonyl compounds.

3.3 Ionisation techniques - Principle of Electrospray ionisation (ESI)-MS, Matrix-assisted laser desorption/ionisation (MALDI)-MS and Fast atom bombardment (FAB)-MS.

Unit 4 : NMR and EPR spectroscopy (1+24+1h)

4.1 Theory of Nuclear magnetic resonance (NMR) spectroscopy - nuclear spin, magnetic nuclei, nuclear magnetic moment, NMR transition, Bloch equations, relaxation mechanisms.

4.2 Parameters of NMR - chemical shift, shielding and deshielding, factors affecting chemical shift-inductive effect, anisotropy, hydrogen bond. Region of proton chemical shift inorganic molecules, chemical shift equivalence and magnetic equivalence. NMR of paramagnetic compounds: Shift reagents in NMR.

4.3 Spin-spin splitting - mechanism and application to structure determination. Coupling constants: mechanism of coupling, first order patterns, second order effects, examples of AB, AX, ABX systems, geminal coupling, vicinal coupling, variation of coupling constants with bond angle, dihedral angle. Long-range coupling, aromatic coupling, virtual coupling.

4.4 Fourier Transform (FT) and 2D NMR spectroscopy : Principle of FT-NMR, Free induction decay (FID). Introduction of 2D techniques: Correlation spectroscopy (COSY), Nuclear overhauser effect spectroscopy (NOESY) and Hetero-COSY. ^{13}C, ^{19}F and ^{31}P NMR spectra of typical examples. Principle of solid state NMR.

4.5 Electron paramagnetic resonance (EPR) spectroscopy - theory of EPR, presentation of the spectrum, nuclear hyperfine splitting in isotropic systems.

4.6 EPR spectra of anisotropic systems - anisotropy in g-value, causes of anisotropy, anisotropy in hyperfine coupling, hyperfine splitting caused by quadrupole nuclei. EPR spectra of systems with more than one unpaired electrons: Zero-field splitting (ZFS), causes of ZFS, ZFS and EPR transitions. EPR of triplet naphthalene, copper salen complex and high-spin Mn(II) complexes.

4.7 Structural elucidation of organic compounds by combined spectral techniques.

Unit-5: NQR and Mossbauer Spectroscopy (1+10+1h)

5.1 Principle of Nuclear quadrupole resonance (NQR) spectroscopy - nuclear charge distribution and quadrupole moment, quadrupole nucleus and its interaction with electric field gradient, nuclear orientations, asymmetry parameter, quadrupole energy levels, transitions in spherical and axially symmetric fields, effect of magnetic field.

5.2 Applications of NQR spectroscopy : quadrupole coupling constant and its interpretation, structural information from NQR spectra of haloorganic compounds, point group symmetry, phase transitions, chemical bonding and hydrogen bonding.

5.3 Principle of Mossbauer spectroscopy : Doppler shift, recoil energy. Isomer shift, quadrupole splitting, magnetic interactions. Applications: Mossbauer spectra of high and low-spin Fe and Sn compounds.

Text books

1. C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 4th Ed., TataMcGraw Hill, New Delhi, 2000.
2. R. M. Silverstein and F. X. Webster, *Spectroscopic Identification of Organic Compounds*,6th Ed., John Wiley & Sons, New York, 2003.
3. W. Kemp, *Applications of Spectroscopy*, English Language Book Society, 1987.
4. D. H. Williams and I. Fleming, *Spectroscopic Methods in Organic Chemistry*, 4th Ed., TataMcGraw-Hill Publishing Company, New Delhi, 1988.
5. D. Pavia, G. M. Lampman, and G.S. Kriz,*Introduction to Spectroscopy*, 3rd Ed., JohnVondeling, Florida, 2006.

6. K. V. Raman, R. Gopalan and P. S. Raghavan, *Molecular Spectroscopy*, Thomson and VijayNicole, Singapore, 2004.
7. R. S. Drago, *PhysicaI Methods in Chemistry*; Saunders: Philadelphia, 1992.
8. G. M. Bancroft, *Mössbauer spectroscopy*, McGraw Hill, London, 1973.

References

1. P.W. Atkins and J. de Paula, *Physical Chemistry*, 7th Ed., Oxford University Press, Oxford, 2002.
2. I. N. Levine, *Molecular Spectroscopy*, John Wiley & Sons, New York, 1974.
3. A. Rahman, *Nuclear Magnetic Resonance-Basic Principles*, Springer-Verlag, New York,1986.
4. K. Nakamoto, *Infrared and Raman Spectra of Inorganic and coordination Compounds*, PartB: 5th ed., John Wiley& Sons Inc., New York, 1997.
5. J. A. Weil, J. R. Bolton and J. E. Wertz, *Electron Paramagnetic Resonance*; Wiley Interscience, 1994.
6. L.D. Field, S. Sternhell, and J. R. Kalman, *Organic Structures from Spectra*, 3rd Ed., John Wiley & Sons Ltd England, 2003.
7. J. W. Akitt, *NMR and Chemistry*, 3rd,ed., Chapman & Hall, London,1992.
8. Jack K. Becconsall, *Basic one and two dimensional NMR Spectroscopy*, 4thEd., Wiley – VCH,2005.
9. R. V. Parish, *NMR, NQR, EPR, and Mossbauer Spectroscopy in inorganic chemistry*, EllisHorwood, London.
10. A. Abragam, B. Bleaney, *Electron Paramagnetic Resonance of Transition Metal ions*, Oxford University Press, 1970.

16PCH2MC04 ORGANIC LABORATORY TECHNIQUES –II

SEMESTER	**II**	**CREDITS**	**3**
CATEGORY	**MC(L)**	**NO.OF HOURS/ WEEK**	**4**

Objectives

1. To develop analytical skill in organic quantitative analysis.
2. To understand the techniques involved in estimations of organic compounds.

1. Estimations

a) Phenol (bromination)
b) Aniline(bromination)
c) Ethyl methyl ketone (iodimetry)
d) Glucose (redox)
e) Ascorbic acid (iodimetry)
f) Aromatic nitro groups (reduction)
g) Glycine (acidimetry)

2. Extraction

a) Caffeme from tea leaves
b) Nicotine from tobacco leaves
c) Citric acid from citrus fruits
d) Lycopene from tomatoes.

3. Separation of components of a mixture (Demonstration)

a) Thin layer chromatography
b) Column chromatography
c) Paper chromatography.

Text books

1. N. S. Gnanapragasam and G. Ramamurthy, *Organic Chemistry – Lab manual*, S. Viswanathan Co. Pvt. Ltd, 1998.
2. J. N. Gurtu and R. Kapoor, *Advanced Experimental Chemistry*, S. Chand and Co., 1987.

Reference

1. Vogel's *Text book of Practical Organic Chemistry,* 5th Ed, ELBS/Longman, England, 1984.

16PCH2MC05 INORGANIC SEMIMICRO QUALITATIVE ANALYSIS

SEMESTER	**II**	**CREDITS**	**4**
CATEGORY	**MC(L)**	**NO.OF HOURS/ WEEK**	**6**

Objectives

1. To study the principle of distribution of common and rare metal ions in different groups.
2. To know inter- and intra-group precipitation and separation of metal ions.
3. To improve the skill in the qualitative analysis of rare metal ions in different groups.
4. To identify the methodology to analyse a metal ion in the presence of another metal ion.

1. Theoretical Principles

1.1 Classification of cations into groups, group reagents.

1.2 Inter group and intragroup separations.

1.3 Confirmatory test for cations-the reaction and the product.

2. Analysis of mixture of cations

Analysis of a mixture of four cations containing two common and two rare.

Cations to be tested.

Group-I	: W, Tl and Pb.
Group-II	: Se, Te, Mo, Cu, Bi and Cd.
Group-III	: Tl, Ce, Th, Zr, V, Cr, Fe, Ti and U.
Group-IV	: Zn, Ni, Co and Mn.
Group-V	: Ca, Ba and Sr.
Group-VI	: Li and Mg.

Text Books

1. V. V. Ramanujam, *Inorganic Semimicro Qualitative Analysis*; 3rd ed., The National Publishing Company, Chennai, 1974.
2. *Vogel's Text book of Inorganic Qualitative Analysis,* 4th ed., ELBS, London, 1974.

16PCH2ES01 BIOMOLECULES AND NATURAL PRODUCTS

SEMESTER	**II**	**CREDITS**	**3**
CATEGORY	**ES (T)**	**NO.OF HOURS/ WEEK**	**4**

Objective

1. To enable the student to understand and appreciate the importance of biomolecules.
2. To understand the techniques involved in the extraction and methods of determination of structure of natural products.

Unit-1: Carbohydrates and Lipids (1+10+1 h)

1.1 Carbohydrates: Synthesis of glycosides, amino sugars, sucrose and maltose.
1.2 Biological importance of glycosides, amino sugars, sucrose, maltose cellulose, starch, glycogen, dextran, hemicellulose, pectin, agar-agar, chitosan, and chrysin.
1.3 Carbohydrate metabolism: glycolysis and gluconeogenesis, pentose phosphate pathway, Carbohydrate in plants and bacteria, tricarboxylic acid (TCA) cycle. Relation between glycolysis and respiration.
1.4 Lipids: synthesis and degradation of neutral lipids, Phospho lipids (lecithines, cephalins, plasmalogens) and glycolipids.
1.5 Lipid Metabolism: Oxidation of glycerol – β-oxidation of fatty acids; Fatty acid metabolism: Regulation of fatty acid metabolism; Allosteric regulation.

Unit-2: Proteins and nucleic acids (1+10+1 h)

2.1 Separation and purification of proteins – dialysis; gel filtration - electrophoresis. Catabolism of amino acids: transamination, oxidative deamination and decarboxylation. Biosynthesis of proteins: Role of nucleic acids. Amino acid metabolism; the urea cycle

2.2 Structure and synthesis of nucleosides and nucleotides; Structure of RNA and DNA, Watson-Crick model; Solid phase synthesis of oligonucleotides.

2.3 DNA intercalators; Chemical synthesis of DNA; Catalytic RNA, siRNA; micro RNA; Synthesis and Application of Unnatural Nucleosides; Fluorescently Labeled Nucleosides and oligonucleotide probes; Single Nucleotide Polymorphism (SNPs).

Unit–3: Vitamins, Hormones and antioxidants (1+12+1 h)

3.1 Vitamins: Types, structure discussion, properties and biological importance of Vitamin A, Vitamin B complex: B_1, B_{12}, Folic acid, Vitamins C, D and E.

3.2 Hormones: Introduction, classification, Sex hormones: Androgens and estrogens. Synthesis and functions. Adrenocortical hormones: Cartisone and aldosterone. Non steroidal Hormones: Adrenaline and thyroxin. Effects of hormone activity on biological functions.

3.3 Antioxidants: Nutrients with an antioxidant role, the need for biological antioxidants, pro-oxidant activity of biological antioxidants, Nutrients associated with endogenous antioxidant mechanisms, Nutrients with radical-quenching properties, β-Carotene and other carotenoids, requirement for antioxidant nutrients.

3.4 Free radicals induced damages, lipid peroxidation, measurement of free radicals, disease caused by radicals, reactive oxygen species, antioxidant defence system, enzymic and non-enzymic antioxidants, role of antioxidants in prevention of diseases, phytochemicals as antioxidants.

Unit-4: Alkaloids (1+9+1 h)

4.1 Classification and isolation. General methods of structural elucidation of alkaloids.

4.2 The structural elucidation of Belladine, Papaverine, Cocaine, Atropine, Heptaphylline, and Peepuloidin. Morphine – Structure and biological functions (SAR).

Unit-5: Terpenoids and carotenoids (1+9+1 h)

5.1 Classification and isolation. General methods of determination of structure.

5.2 Structural elucidation of Cadinene, Vitamin A, β-carotene, Abietic acid, Gibberelic acid, Zinziberine and Squalene.

Text books

1. T. K Lindhorst, *Essentials of Carbohydrate Chemistry and Biochemistry*, Wiley VCH,North America, 2007.
2. G. K. Chatwal, *Organic Chemistry on Natural Products,* Vol. 1, Himalaya Publishing House, Mumbai, 2009.
3. G. K. Chatwal, *Organic Chemistry on Natural Products, Vol. 2,* Himalaya Publishing House, Mumbai, 2009.
4. O. P. Agarwal, *Chemistry of Organic Natural Products, Vol. 1,* Goel Publishing House, Meerut, 1997.
5. O. P. Agarwal, *Chemistry of Organic Natural Products, Vol. 2*, Goel Publishing House, Meerut, 1997.
6. I. L. *Finar, Organic Chemistry Vol-2, 5th ed., Pearson* Education Asia, 1975.
7. V. K. Ahluwalia and M. Goyal, Textbook of Organic Chemistry, Narosa Publishing, New Delhi, 2000.

References

1. I. L. Finar, *Organic Chemistry Vol-1, 6th ed.*, Pearson Education Asia, 2004.
2. Pelletier, *Chemistry of alkaloids*, Van Nostrand Reinhold Co, 2000.
3. Shoppe, *Chemistry of the steroids*, Butterworthes, 1994.

4. I. A. Khan, and A. Khanum. Role of Biotechnology in medicinal & aromatic plants, Vol 1 and Vol 10, Ukkaz Publications, Hyderabad, 2004.
5. M. P. Singh. and H. Panda, Medicinal Herbs with their formulations, Daya Publishing House, Delhi, 2005.
6. V. K. Ahluwalia, Steroids and Hormones, Ane books pub., New Delhi, 2009.

16PCH2ES02 SURFACE CHEMISTRY AND CATALYSIS

SEMESTER	**II**	**CREDITS**	**3**
CATEGORY	**ES(T)**	**NO.OF HOURS/ WEEK**	**4**

Objectives

1. To understand the basic concepts of surface chemistry and colloids.
2. To know the different methods of catalysis
3. To learn the various techniques and mechanisms involved in catalysis.

Unit 1: Adsorption (1+8+1 h)

1.1 Fundamental concepts – surface tension, curved surfaces, capillary action. Adsorption- factors affecting adsorption.
1.2 Unimolecular adsorption – Freundlich, Langmuir – simple, dissociation, competitive and non-ideal adsorption, Multimolecular adsorption: Brunauer-Emmett and Teller, Harkins-Jura equations. Types of adsorption isotherms.
1.3 Adsorption from solution- Gibbs adsorption isotherm, surface films.
1.4 Kinetics of bimolecular reactions on surfaces: Eley-Rideal and Langmuir-Hinshelwood mechanisms.

Unit 2: Colloids (1+8+1 h)

2.1 Surfactants – anionic, cationic and amphoteric, hydrophile-lipophile balance.

2.2 Micelles – formation, critical micellar concentration (CMC), factors affecting CMC in aqueous media, micellar catalysis.
2.3 Uses of CMC for the synthesis of zeolites, mesoporous and metal organic framework materials.
2.4 Emulsions – micro and macro, selection of surfactants as emulsifiers, preparation; elastic and non-elastic gels.

Unit 3: **Homogeneous and Heterogeneous catalysis** (1+13+1 h)

3.1 Introduction to catalysis - activity, selectivity, promoters, stabilisers and poisons, catalysts deactivation, auto catalysts, turnover number and inhibitors.
3.2 Homogeneous catalysed reactions – general mechanism, activation energy for the process, acid-base catalysis – catalytic activity, acid-base strength, acidity functions. Homogeneous catalysts for the polymerization of olefins, oxidative dehydrogenation, ethyl benzene to styrene.
3.3 Steps involved in heterogeneous catalysis, thermodynamic considerations. Preparation of catalysts – precipitation and impregnation methods. Role and load of supports. Heterogeneous catalysts for catalytic cracking and Fischer-Tropsch synthesis.

Unit 4: Photo and Bio Catalysis (1+12+1 h)

4.1 Photocatalysis: n- and p-type and metallised semiconductors as photocatalysts (TiO_2 and ZnO) – application for the degradation of dyes, solar energy conversion, electrochemical cells, photoelectrolysis of water. Photocatalysis for organic reactions-oxidation, reduction, polymerization, substitution and isomerization reaction using TiO_2.
4.2 Biocatalysis – Mechanisms - covalent catalysis, acid-base and metal-ion catalysis, entropy and geometric effects, structural complementary of the active site to the transition state, prevention of the side reactions, the size of the enzymes. Application of enzymes in organic

synthesis - Oxidoreductase: Oxidation - alcohols, epoxides, sulfoxides, amino acids, lactones; Reduction: α- hydroxyl aminoacid; Transferase-amino acids, amines.

Unit 5: Surface Characterisation Techniques (1+9+1 h)

5.1 Surface area determination – BET, pore volume, and pore size distribution-BJH and t-plot methods.

5.2 Thermal methods – temperature programmed desorption and reduction.

5.3 Spectroscopic techniques: X-ray photoelectron spectroscopy, Auger electron spectroscopy, surface plasmon resonance, X-ray fluorescence spectroscopy – Principle and applications in surface analysis.

Text Books

1. K.J. Laidler, *Chemical Kinetics*, 3rd edition, Pearson, Reprint 2013.
2. B. Viswanathan, S. Sivasanker and A.V. Ramaswamy, *Catalysis: Principles and Applications*, Narosa Publishing House, New Delhi, 2004.
3. D. K. Chakrabarthy and B. Viswanathan, *Heterogeneous catalysis*, New Age International Publishers, 2011.
4. B.R. Puri, L.R. Sharma and M.S.Pathania, *Principles of physical chemistry*, ShobanLalNagin Chand and Co. 46th edition, 2013.

Reference Books

1. J. Rajaram and J.C. Kuriokose, *Kinetics and Mechanisms of chemical transformation*, Macmillan India Ltd, 2011.
2. G.C. Bond, Heterogeneous catalysis: Principles and applications, Oxford University Press, Ely House, London W.I, 1974.
3. V.Murugesan, A. Banumathi and M. Palanichamy, *Recent Trends in Catalysis*, Narosa Publishing House, New Delhi, 1999.

4. C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 4th Ed., TataMcGraw Hill, New Delhi, 2000.

16PHE2FC01 LIFE SKILLS TRAINING

SEMESTER	**II**	**CREDITS**	**2**
CATEGORY	**FC(T)**	**NO.OF HOURS/ WEEK**	**2+2**

OBJECTIVES OF PG SYLLUBUS

1. To improve and sustain the primal level of competence and performance of PG students through an advanced training of holistic development of oneself.
2. To empower through various skills and strengthen them to face the future life issues and challenges.
3. To equip them with practical and value based learning of soft skills for a better life in future.

INSIDE CLASS HOURS (2 hrs)

Unit – I: Constructing Identity

Self Image – Understanding self image – shadows down the lane – self acceptance **- Self Knowledge** – Knowing oneself **- Self confidence –** Guilt and grudges - Power of belief – positive thinking– optimizing confidence **- Self development –** perception, attitude and Behavioural change, developing a healthy and balance personality **- Self esteem –** signs - indicators

Unit – II: Capacity Building

Motivation – Definition, types (Intrinsic and Extrinsic), Theories (Maslow's hierarchical needs, etc), Factors that affect motivation, Challenges to motivation, Strategies to keep motivated, motivational plan. **Time Management Skills–** steps to improve time management, overcoming procrastination, assessing and planning weekly schedule, challenges, goal settings, components of goal settings, consequences of poor time management, control of interruption and distractions. Communication, public speaking, talents, creativity, learning,

Unit – III: Professional Skills

-Leadership development skills – difference between leader and manager, different styles and their utilities, functions of leadership, application of knowledge, overcoming from obstacles, influential skills and Leadership qualities. **Application skills** – Managing Career and self-direction, Visionary thinking, formulating strategies, shaping strategies, building organizations relationships, change management. Project Management Skills, Independent working skills, Writing skills, Public Speaking, analytical Skills, Neo Research and Development. **Problem solving skills** – Process, approaches and its components, creative problem solving, Tools and techniques, application of SMART analysis and barriers to problem solving.

Unit – IV: Life Coping Skills

Life skills – Personal and reproductive Health, love, sex, marriage and family – family life education – Gender Equity - child bearing and Childrearing practices, Geriatric Care - adjustability **Human Relationship** – formal and informal - peer group – friends – same and other gender - family – Colleagues – community – emotional intelligence - **Stress Coping skills** – Definition of stress, strategies to alleviate stress, problem and emotion focused coping, techniques to reduce stress, stress reaction phases, crisis intervention steps, creating positive affirmations, Signs, Symptoms and Reactions of Stress.

Unit – V: Social Skills

Human Rights Education, Understanding Human Rights, International and national mechanisms, protection and preservation of HRs, Human Rights in the context of new, technological and electronic society, **Peace Education,** Social Harmony in the context of religious fundamentalism and fanaticism, Understanding Peace and Justice, Conflict Resolution Strategies

Reference books

1. Healing Your Emotional Self: A Powerful Program to Help You Raise Your Self-Esteem, Quiet Your Inner Critic, and Overcome Your Shame by Beverly Engel
2. Self-knowledge and self-discipline by B. W. Maturin
3. Motivation: Biological, Psychological, and Environmental (3rd Edition) by Lambert Deckers
4. Getting Things Done: The Art of Stress-Free Productivity by David Allen
5. Managerial Skills in Organizations by Chad T. Lewis
6. Social Intelligence: The New Science of Human Relationships by Daniel Goleman

Competence building	**Career Preparatory Training**
Power talk	Interview Guidance
Emotional Intelligence	Group Dynamics
Stress management	Leadership skills
Decision Making	Negotiation Skills
Positive image building	Creative writing

OUTSIDE THE CLASS HOURS (2 hrs)

- Each student will choose either of the above-mentioned modules and is expected to undergo a training/workshop in that module.
- She/he will have to accomplish ten hrs outside the class hours to fulfill the 2 credits.

Methodology

Inputs, ABL model, Documentaries, group activities and Interaction, Special workshop by professionals.

Evaluation

There will be end test and a Project for 'inside the class hours'. Viva Voce will be conducted for the 'Outside the class hours'.

16PCH3MC01 MAIN GROUP ELEMENTS AND NUCLEAR CHEMSITRY

SEMESTER	**III**	**CREDITS**	**5**
CATEGORY	**MC(T)**	**NO.OF HOURS/ WEEK**	**5**

Objectives

1. To know the structure and bonding in inorganic chains, rings, and cages.
2. To identify ligands of main group elements and complexing agents for main group metals.
3. To identify specific reagents of main-group elements usedin synthesis.
4. To understand theory of radioactivity and applications of radioisotopes.
5. To know the working principle and safety features of nuclear reactors.

Unit-1: Inorganic Chains, Rings, and Cages

1.1 Catenation and hetero catenation: allotropes of carbon, graphite, diamond, fullerenes, carbon nanotubes and graphene. Hetero catenation-by coupling cyclic silicon and phosphorous compounds.

1.2 Alkali and alkaline earth metal complexes: complexes of β-diketones, crown ethers, cryptands, and calixarenes; biological roles of alkali and alkaline earth metal ions and ionophores.

1.3 Electron deficient, electron precise, and electron rich compounds: boranes and carboranes: synthesis of neutral boron hydrides, polyhedral borane anions and dianions, structure of polyhedral boranes- *nido*-, *arachno*-, and *closo*-frameworks, general formula, PSEPT (Wade's rules) and polyhedral geometries; carboranes-synthesis and polyhedral geometries, metalloboranes, and metallocarboranes. Silanes and cyclopolysilanes, hydrometallation-hydroboration and hydrosilylation. Hydroboration reaction as precursor for metalloborane and heteroborane clusters. Styx number. Synthetic importance of diborane, boranes.

Unit-2 Nitrogen and Sulphur Compounds

2.1 Boron-nitrogen compounds: azaboranes, pyrazaboles, borazines, and B-N clusters.

2.2 Silicates: classification-orthosilicates, noncyclic silicate anions, cyclic silicate anions, infinite chain anions, infinite sheet anions, framework minerals, and zeolites-typical examples and structure, cyclic siloxanes

2.3 Poly acids: structure of isopoly and heteropoly anions and polycations of W and Mo.

2.4 P-N and P-S compounds: polyphosphazene, cyclophosphazenes, and cyclic aminophosphanes, phosphorus-oxide and phosphorus-sulfide cages.

2.5 Cyclic sulfur-nitrogen compounds: tetrasulfur-tetranitride, polythiazyl, and S_xN_y compounds.

Unit-3: Main Group Organometallics and Reagents

3.1 Organometallic compounds of Li, Be, and Mg: synthesis and applications. Organometallic reagents-structure and bonding.

3.2 Organometallic compounds of Si and Al: silsesquioxanes, aryl- and alkyl silicon halides, aluminium alkyls.

3.3 Specific reagents of main-group elements: fluorinating agents-ClF, ClF_3, and BrF_3 (harsh); SF_4, SbF_3, and SbF_5 (moderate)

3.4 Special techniques for the synthesis of air sensitive compounds: the vacuum line, plasmas, photochemical apparatus, and electrolysis. Synthetic importance of PCl_3, and silylating agents. Drying of solvents.

Unit-4: Halogen and Noble Gas Chemistry

4.1 Halogen oxides and oxo compounds: Dichlorine monoxide, chlorine dioxide, dibromine monoxide, and iodine pentoxide-preparation and properties; halogen oxyfluorides trioxohalo fluorides) and ionic oxyhalogen species.

4.2 Xenon oxides and fluorides: xenon trioxide, difluoride, tetrafluoride, xenon oxofluoride.

4.3 Halogen compounds of nitrogen: nitrogen trifluoride, tetrafluoro hydrazine, dinitrogen difluoride, haloamines, oxohalides, and nitrogen trifluoride oxide.

4.4 Sulfur fluorides: Synthesis and reactivity of disulfur difluoride, sulfur tetrafluoride, substituted sulfur fluorides.

4.5 Structure of halogen oxides and halogen oxo compounds with the aid of VSEPR model. Reactivity of the halides of N, S, and Xe and applications.

Unit-5: Radiochemistry and Nuclear Reactions

5.1 Introduction. Types of nuclear reactions: Spallation, fusion-hydrogen bomb, stellar energy, nuclear fission-theory of nuclear fission; chain reaction, nuclear cross section, critical mass; atom bombs, nuclear fission reactors, breeder reactors-fuels used in nuclear reactors, moderators, coolants; nuclear fusion; separation of isotopes, nuclear reactors in India.

5.2 Measurement of radioactivity: ionization chamber, GM counters, scintillation counters.

5.3 Reprocessing of spent fuels: Nuclear waste streams from nuclear reactors, sequestering agents for radioisotopes, solvent extraction and ionic liquid technology.

5.4 Applications: Dating of objects-principles, ^{14}C dating (specific examples) and applications, neutron activation analysis, isotopic dilution and labeling studies, nuclear medicine-^{99m}Tc radiopharmaceuticals.

5.5 Isotopes used in nuclear fission reactions. Use of radioisotopes in noninvasive imaging techniques and in nuclear medicine.

Text books

1. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*; 6th ed.; Wiley Interscience: New York, 1988.
2. J. E. Huheey, E. A. Keiter and R. L. Keiter, *Inorganic Chemistry*; 4th ed.; Harper and Row: New York, 1983.
3. D. F. Shriver, P.W. Atkins and C.H. Langford, *Inorganic Chemistry*; 3rd ed.; Oxford University Press: London, 2001.
4. K. F. Purcell and J. C. Kotz, *Inorganic Chemistry*, Saunders: Philadelphia, 1976.

References

1. T. Moeller, *Inorganic Chemistry, A Modern Introduction*; John Wiley: New York, 1982.
2. H. J. Arnikar, *Essentials of Nuclear Chemistry*; 4th ed., New Age International, New Delhi, 1995.
3. A. K. Srivatsava and P. Jain, P. *Essential of Nuclear Chemistry*; S. Chand, New Delhi, 1989.
4. G. Friedlander, G.; Kennedy, W. and J. M. Miller, *Nuclear and Radiochemistry*; 2nd ed.; John Wiley and Sons Inc., 1964.
5. S. Glasstone, *Source Book on Atomic Energy*; 2nd ed.; Van Nostr and Co. Inc., New Jersey, 1958.

16PCH3MC02 THERMODYNAMICS AND CHEMICAL KINETICS

SEMESTER	**III**	**CREDITS**	**5**
CATEGORY	**MC(T)**	**NO.OF HOURS/ WEEK**	**6**

Objectives

1. To know the limitations of quantum chemistry and classical thermodynamics in the evaluation of macroscopic properties.
2. To understand the inter linking of quantum chemistry and statistical thermodynamics that leads to classical thermodynamics.
3. To apply the concepts of statistical thermodynamics for the study of equilibrium reactions and reaction rates

Unit 1: Classical Thermodynamics (1+16+1 h)

1.1 Thermodynamic systems of variable composition: Partial molal quantities - Chemical potential. Gibbs-Duhem equation. Determination of partial molal quantities. Ellingham diagram and its significances.

1.2 Thermodynamics of real gases and real solutions: Fugacity: Methods of determination. Dependence on temperature, pressure and composition. Activity and activity coefficient: Standard states, determination of activity and activity coefficient of non-electrolytes and electrolytes.

1.3 Ternary systems involving three liquids. Solubility of ionic solids in water-Solubility curves. Ternary system involving water and two soluble ionic solids. Formation of double salts.

Unit2: Irreversible Thermodynamics (1+10+1 h)

2.1 Near equilibrium process: General theory- Conservation of mass and energy- Entropy production in open system by heat, matter and current flow; Force and flux.

2.2 Onsager theory: Validity and verification – Principle of microscopic reversibility, Onsager reciprocal relations.

2.3 Thermoelectricity-Electro kinetic and thermo mechanical effects

2.4 Application of irreversible thermodynamics to biological and non-linear systems.

Unit 3: Statistical Concepts of Thermodynamics(1+13+1 h)

3.1 Macro and micro states: Distribution of particles in different energy levels. Maxwell- Boltzmann statistics. Distribution of molecular velocities.

3.2 Partition functions: Canonical and molecular partition functions. Separation of partition functions. Translational, rotational, vibrational and electronic partition functions. Interpretation of partition function.

3.3 Statistical approach to Thermodynamic properties: Internal energy, entropy, enthalpy, Helmholtz function, pressure, Gibbs function, residual entropy, equilibrium constant, average energies and equipartition principle. Heat capacity of mono and diatomic gases. Ortho- and para hydrogen, heat capacity of solids- Einstein and Debye models.

3.4 Quantum Statistics Bose-Einstein statistics-Theory of paramagnetism. Statistics of a photon gas and liquid helium.Fermi-Dirac statistics-Thermionic emission-Electron gas (metals).

3.5 Statistical approach to equilibrium constants – Free energy function

Unit 4: **Kinetics of reactions in gas phase and in solutions and catalysis** (1+23+1 h)

4.1 Theories of reaction rates - Kinetic theory of collisions – bimolecular, unimolecular - Lindemann - Christiansen hypothesis, Hinshelwood treatment, bimolecular reactions in gas phase (involving atoms and free radicals) potential energy surface. Conventional transition state theory -Evaluation of thermodynamic parameters of activation, application of ARRT to reactions between atoms, molecules and atoms & molecules- time and true order.

4.2 Factors determining reaction rates in solution - ionic strength - primary and secondary salt effects, dielectric constant – concept of electrostriction, hydrostatic pressure - volume of activation.

4.3 General catalytic mechanisms. Equilibrium and steady state treatments. Enzyme catalysis - Michalis-Menten equation-evaluation of kinetic parameters, Turn over number. Enzyme inhibition - Kinetics of enzyme inhibition – competitive, uncompetitive and non - competitive, degree of inhibition. Bimolecular reactions on surfaces - Eley-Rideal and Langmuir-Hinshelwood mechanisms.

Unit 5: **Kinetics of Complex and fast Reactions** (1+18+1 h)

5.1 Rate expressions for opposing, parallel and consecutive reactions; Chain reactions – chain length, Rice-Herzfeld pyrolysis of acetaldehyde, hydrogen-halogen (thermal and photochemical) reaction, Gas phase auto oxidation; explosion and explosion limits.

5.2 Kinetics and mechanism of polymerisation reactions: free radical, cationic and anionic –chain initiation – propagation –termination –chain transfer – inhibition and retardation.

5.3 Flow techniques - relaxation theory and relaxation techniques - Temperature, Pressure, electric field and magnetic field jump methods; Flash photolysis and pulse radiolysis.

Text Books

1. J. Rajaram and J.C. Kuriacose, Thermodynamics For Students of Chemistry, 2nd edition, S.L.N. Chand and Co., Jalandhar, 1986.
2. I.M. Klotz and R.M. Rosenberg, Chemical thermodynamics, 6th edition., W.A.Benjamin Publishers, California, 1972.
3. M.C. Gupta, Statistical Thermodynamics, New Age International, Pvt. Ltd., New Delhi, 1995.

4 K.J. Laidler, Chemical Kinetics, 3rd edition, Pearson, Reprint - 2013.
5. J. Rajaram and J.C. Kuriokose, Kinetics and Mechanisms of chemical transformation, Macmillan India Ltd, Reprint - 2011.
6. V.R. Gowariker, Polymer Science, Wiley Eastern, 1995.

References

1. D.A. McQurrie and J.D. Simon, Physical Chemistry - A Molecular Approach, Viva Books Pvt. Ltd., New Delhi, 1999.
2. R.P. Rastogi and R.R. Misra, Classical Thermodynamics, Vikas Publishing, Pvt. Ltd., New Delhi, 1990.
3. S.H. Maron and J.B. Lando, Fundamentals of Physical chemistry, MacMillan Publishers, New York, 1974
4. K.B. Ytsiimiriski, " Kinetic Methods of Analysis", Pergamom press,1996.
5. K.K.Rohatgi Mukherjee, "Fundamentals of Photochemistry", Revised edition, New Age International Publishers, New Delhi, 1978.

16PCH3MC03 SCIENTIFIC RESEARCH METHODOLOGY AND COMMUNICATIONS

SEMESTER	**III**	**CREDITS**	**3**
CATEGORY	**MC(T)**	**NO.OF HOURS/ WEEK**	**4**

Objectives

1. To introduce the purpose and importance of research for future development.
2. To know the various indexes and abstracts in science and technology.
3. To learn literature search for current awareness and for retrospective survey.
4. To know the methodology of writing thesis and journal articles.

Unit-1: Meaning of Research (1+9+1 h)

1.1 The search for knowledge, purpose of research, nature of scientific knowledge, scientific method, role of theory, characteristics of research. Types of research: fundamental or pure research, applied research, action research, historical research, experimental research.

1.2 Assessment and evaluation-purpose and general methodology.

Unit-2: The Chemical Literature (1+11+1 h)

2.1 Sources of chemical information: primary, secondary and tertiary sources. Indexes and abstracts in science and technology.

2.2 Classical and comprehensive reference works in chemistry: Beilstein's Handbook of Organic Chemistry, Dictionary of Organic Compounds, Merck Index, CRC Handbook of Chemistry and physics. Reviews: Annual and quarterly reviews, general reviews.

Unit-3: The Chemical abstract services (1+8+1 h)

3.1 The Chemical Abstracts: Current awareness searching: CA weekly issues, CA issue indexes. Retrospective and forward searching. CA Collective indexes: Collective index (CI), decennial index (DI).

3.2 Access points for searching CA indexes: index guide, general subject terms, chemical substance names, molecular formula, ring systems, author names, patent numbers. Locating the reference: finding the abstract, finding the original document, chemical abstract service source index.

3.3 Online Searches: ASAP Alerts, CA Alerts, SciFinder, ChemPort, Sciencedirect, STN International. Google scholar, Scopus international.

3.4 Journal home pages.

Unit-4: The Scientific Writing **(**1+13+1 h)

4.1 Scientific writings: research reports, thesis, and journal articles. Requirement of technical communications:

eliminating wordiness and jargon-tautology, redundancy, imprecise words, superfluous phrases. Lab notebook maintenance.

4.2 Steps to publishing scientific articles in journals: types of publications-communications, articles, reviews; where to publish, specific format required for submission, organization of the material.

4.3 Documenting: abstracts-indicative or descriptive abstract, informative abstract, footnotes, end notes, referencing styles, bibliography-journal abbreviations (CASSI), abbreviations used in scientific writing.

Unit-5: Seminar-Scientific Communication **(**1+9+1 h)

5.1 *Recent Advancements in Chemistry*: Supramolecular Chemistry, Green Chemistry, Material Chemistry, Organic Synthesis, Nano materials, chemistry,

Text Books

1. B. E. Cain, *The Basis of Technical Communicating*, ACS., Washington, D.C., 1988.
2. J. W. Best, *Research in Education*, 4th ed. Prentice Hall of India, New Delhi, 1981.
3. H. F. Ebel, C. Bliefert and W. E. Russey, *The Art of Scientific Writing*, VCH, Weinheim, 1988.
4. J. Gibaldi, and W. S. Achtert, *Handbook for Writers of Research Papers*; 2nd ed.; Wiley Eastern, 1987.
5. A. Joseph, *Methodology for Research*; Theological Publications, Bangalore, 1986.

References

1. R. L. Dominoswki, *Research Methods*, Prentice Hall of India, New Delhi, 1981.
2. H. M. Kanare, *Writing the Laboratory Notebook*; American Chemical Society: Washington, DC, 1985.
3. J. S. Dodd, Ed., *The ACS Style Guide: A Manual for Authors and Editors*; American Chemical Society: Washington, DC, 1985.

16PCH3MC04 PHYSICAL

CHEMISTRY PRACTICAL –I

SEMESTER	**III**	**CREDITS**	**3**
CATEGORY	**MC(L)**	**NO.OF HOURS/ WEEK**	**4**

Objectives

The students will be able to

1. apply the concepts of equilibrium, thermodynamics, phase rule and colligative properties to various experiments.
2. acquire analytical skills for quantitative analysis.

Experiments

1. Verification of Freundlich adsorption isotherm – Study of adsorption acetic acid or oxalic acid on charcoal and determination of concentration of the given acid.
2. Construction of Phase diagram for two components – Compound forming systems: Diphenylamine – Benzophenone.
3. Determination of equilibrium constant for the formation of potassium triiodide from iodine and KI and the concentration of unknown potassium iodide solution.
4. Comparison of acid strengths using acid catalysed hydrolysis of methyl acetate.
5. Determination of rate constant and order for the reaction between potassium persulphate and potassium iodide and determine the temperature coefficient and energy of activation.
6. Kinetic study of acetone and iodine in acidic medium and the determination of order with respect to acetone and iodine.
7. Determination of order of saponification of ethyl acetate by sodium hydroxide.
8. Study the primary salt effect on the kinetics of ionic reactions and test the Bronsted relationship (iodide ion is oxidized by persulphate ion).

9. Determination of energy of activation for the acid catalysed hydrolysis of methyl acetate.
10. Kinetics of inversion of cane sugar-determination of the pseudo first order rate constants using polarimeter.
11. Determination of molar refractions of pure liquids and estimation of concentration of glucose using Abbe's refractometer.
12. Determination of heat of solution of oxalic acid from solubility and thermometric measurements.
13. Determination of the molecular weight of polymer by viscometer.

Text Books

1. B. Viswanathan and P.S.Raghavan, Practical Physical Chemistry, Viva Books, New Delhi, 2009.
2. Sundaram, Krishnan, Raghavan, Practical Chemistry (Part II), S. Viswanathan Co. Pvt., 1996.

References

1. J. B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.
2. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th edition, McGraw Hill, 2009.
3. J. N. Gurthu and R. Kapoor, Advanced Experimental Chemistry, S. Chand and Co., 1987.

16PCH3ES01 APPLIED ORGANIC CHEMISTRY

SEMESTER	**III**	**CREDITS**	**3**
CATEGORY	**ES(T)**	**NO.OF HOURS/ WEEK**	**4**

Objectives

1. To understand the elements of chemical engineering in organic synthesis
2. To appreciate the techniques involved in environment friendly organic synthesis

Unit -1: Organic Chemical Technology (1+13+1 h)

1.1 Unit operations in chemical engineering: Fluid flow: Reynold's number; Bernoullis' equation, Turbulent flow. Mass transfer: Distillation - two and three component systems. Leaching and extraction; stirrers and driers.

1.2 Energy balance over a flow system, heat of reaction, Chemical equilibrium, entropy changes, vapour phase and liquid phase catalytic reactions.

1.3 Factors affecting chemical process kinetics, scaling up of reactions from laboratory to pilot plant to main plant; Materials of construction; Study of industrial scale nitration, sulphonation and halogenations reactions.

1.4 Quality control, R & D, standardization.

Unit-2: Organometallic Compounds (1+8+1 h)

2.1 Synthesis and reactions involving organolithium (n-BuLi, PhLi), organocadmium, organomagnesium, organopalladium, organoselenium, organocobalt, organoaluminium, and organocopper.

2.2 Reactions promoted by samarium diiodide and dicyclopentadienyl samarium – Barbier type reaction, ketyl-alkene coupling reactions, pinacolic coupling reactions, acyl anion reactions and McMurray olefination.

Unit-3: Polymer supported Reagents in Organic Synthesis (1+8+1 h)

3.1 Introduction, choice of polymers, properties and advantages of polymer support and reagents.

3.2 Intramolecular cyclization reactions, bromination by using poly-N-bromosuccinimide, use of polystyrene carbodiimide.

3.3 Acylation with polystyrene anhydride, diazotransfer reaction, Wittig reactions, alkylation, oxidation with peracid and chromic acid, use of polymer supported photosensitizers.

Unit-4: Green Chemistry, (1+8+1 h)

4.1 Green methods, green products, recycling waste. Twelve principles of green chemistry.

4.2 Designing green synthesis-Green reagents: dimethyl carbonate, polymer supported reagents. Green solvents: water, ionic liquids, deep eutectic solvents, supercritical carbon dioxide. Solid state reactions: solid phase synthesis, solid supported synthesis.

Unit-5: Microwave Synthesis, Sonochemistry and Phase Transfer reactions (1+13+1 h)

5.1 Microwave assisted synthesis: Principle, instrumentation, types, limitations and precautions. Applications: Esterification, deprotection of esters and ethers, C- and N-alkylation and condensation of active methylene compounds, rearrangement reactions, synthesis of enamino-ketones and electrophilic alkenes.

5.2 Sonochemistry: Principle, instrumentation, types and precautions. Applications: Esterification, hydrolysis, substitution and addition reactions, oxidation and reduction reactions, coupling reactions.

5.3 Types of phase transfer catalysts, Mechanism and advantages, Preparation of quaternary ammonium salts and crown ethers. Application: Substitution, esterification, addition, condensation and polymerization reactions.

Text books

1. W. L. McCabe, J.C. Smith and P. Harriott, *Unit Operations of Chemical Engineering*, *7th Edn*., McGraw-Hill, New Delhi,2005.
2. J. M. Swan and D. St. C. Black, *Organometallics in Organic Synthesis*, Chapman Hall, 1974.
3. V. K. Ahluwalia and R. Aggarwal, *Organic Synthesis: Special Techniques*, Narosa Publishing House, New Delhi, 2001.

4. K. Tanaka, *Solvent Free Organic Synthesis*, Wiley VCH, Weinheim, 2003.

References

1. P. H. Groggins, *Unit Processes in Organic Synthesis, 5th Edn.*, Tata McGraw Hill, New York, 1995.,
2. C. E. Dridens, *Outlines of Chemical Technology*, Affiliated East-West Press Pvt. Ltd, 2001.
3. C. A. Clausen and G. Matson, *Principles of Industrial Chemistry*, John Willey & Sons, New York, 1978.
4. M. Larhed, and K. Olofsson, *Topics in current chemistry*, Springer, *266*, 2006
5. R. Sanghi and M. M. Srivastava, *Green chemistry, Environment Friendly Alternatives*, Narosa Publishing House, 2007.
6. V. K. Ahluwalia, *Green Chemistry*, Ane Books Pvt. Ltd., 2006.
7. B. Michael Smith, *Organic synthesis*, McGraw Hill International Edition 1994.
8. *Methods and Reagents in Green Chemistry*, Edited by P. Tundo, A. Perosa and F. Zacchini, Wiley-Interscience, 2007.

16PCH3ES02 PHYSICAL CONCEPTS IN INORGANIC CHEMISTRY

SEMESTER	**III**	**CREDITS**	**3**
CATEGORY	**ES(T)**	**NO.OF HOURS/ WEEK**	**4**

Objectives:

1. To quantify bonding parameters in cubic and distorted geometries from absorption spectra.
2. To identify coordination compounds with noble electrochemical and photochemical properties suitable for the construction of supramolecular assemblies and nanostructures.
3. To understand the importance of inorganic

photosensitizers for solar energy conversion.

4. To familiarize the applications of photochemistry in metal complexes

UNIT-1: Electronic Structure and Geometry of Coordination Compounds (1+12+1 h)

1.1 Electronic spectroscopy of metal complexes: principles, classification of electronic spectra, factors influencing band shape–crystal field spectra of O_h and T_d complexes, Jahn-Teller effect. Spectrochemical series, structural evidence from electronic spectra, evaluation of D_o and D_t values in O_h and T_d complexes of Co(III) and Ni(II), quantification of covalency nephelauxetic ratio.

1.2 Tetragonal distortion in octahedral complexes and evaluation of Dq_{xy} and Dq_z in tetragonally distorted octahedral Co(III) complexes. Causes of tetragonal distortion in transition metal complexes and effect on their electronic spectra.

1.3 Infrared and Raman Spectroscopy-functional group interpretation. Determination of coordination sites and linkage isomers (NO_2^-, SCN^-, ClO_4^-), Assigning denticity of ligands (SO_4^{2-} and CO_3^{2-}), Effect of coordination on ligand vibrations-NH_3, H_2O, glycine, PPh_3, 2,2'-bipyridine, 1,10-phenanthroline.

1.4 Raman effect and molecular structure-CO, HCN, CO_2, N_2O and H_2O. Applications of resonance Raman spectroscopy to structural elucidation of the active sites in heme and non-heme oxygen carriers.

UNIT-2: Spin Resonance Spectroscopy and Characterization of Coordination Compounds (1+11+1 h)

2.1 Nuclear magnetic resonance spectroscopy: NMR spectra of quadrupole nuclei, effect of quadrupole nuclei on spin-spin splitting and hyperfine splitting. NMR of paramagnetic transition metal complexes: scalar shift, pseudo contact shift and covalency. Fluxional isomerism.

2.2 Electron spin resonance spectroscopy: principle-hyperfine and zero field effects, nuclear quadrupole interaction. Interpretation of g in cubic, axial rhombohedral geometry, factors affecting 'g' values. Calculation of $g_\perp$ and $g_\parallel$ (Cobalt complexes)–metal-ligand covalency. Huxional behaviour in coordination compounds.

2.3 EPR spectra of bis(salicylaldimine)copper(II), $[(NH_3)_5\text{–}Co\text{-}O_2\text{-}Co(NH_3)_5]^{5+}$, diethyldithiophosphinato copper(II), Co(II)-phthalocyanin complex, $K_2[IrCl_6]$. Interpretation of 'g' and 'A' values from ESR spectral data in MnF_6^{4-}, CoF_6^{4-} and CrF_6^{3-}. ESR spectra of dinuclear Cu(II) complexes. Nuclear quadrupolar interaction–$CuK_2(SO_4)_2.6H_2O$

2.4 Mossbauer spectroscopy: principle, isomer shift and site symmetry of metal ions in coordination compounds. Applications-low and high spin Fe(II) and Fe(III) complexes, π-bonding effects in iron complexes, spin crossover in Fe(II) complexes. Identification of diamagnetic and covalent compounds - Structural aspects of Iron carbonyls, $Fe[Fe(CN)_6]$, $[Fe_3(CO)_{12}]$, $FeSO_4.7H_2O$, $FeCl_3$, $K_4[Fe(CN)_6]$, $K_3[Fe(CN)_6]$ and Iron-sulphur Proteins. Tin compounds-tin halides and organotin compounds. Iodine compounds-isomer shifts of ^{127}I and ^{129}I-applications to alkali metal iodides and molecular iodine.

UNIT- 3: Electrochemical Studies and Photochemistry

(1+8+1 h)

3.1 Applications of AC polarography-cyclic voltammetry to the study of coordination compounds: computation of electrochemical parameters and evaluation of reversibility. Causes of electrochemical irreversibility and coupled chemical reactions. Spectroelectrochemistry-optically transparent electrodes and cells, chronoabsorptiometry.

3.2 Solar and renewable energy: light-to-chemical energy conversion in lamellar solids and thin films, solar energy conversion by dye-sensitized photovoltaic cells and by coordination compounds anchored onto semiconductor surfaces. Photochemical activation and splitting of water, CO_2 and N_2.

3.3 Photochemistry of lanthanide complexes: A-ET-E processes, NIR-to-visible photon up conversion, nonlinear optical behavior, exciton multiplication and relaxation dynamics in quantum dots and applications. Ru(II) and Os(II) polypyridyl complexes employed in solar energy conversion.

Unit-4 Photochemistry of transition metal complexes (1+9+1 h)

4.1 Adamson's Model, Photoreactions-photoaquation, substitution reactions, photoracemisation reaction of Cr(III), Co(III) and Cu(II) complexes

4.2 Manganese based photo systems for water-splitting.

4.3 Complexes of Rh, Ru, Pd and Pt-photochemical generation of hydrogen from alcohol, photocarbonylation of hydrocarbon, photocatalytic hydrogenation of alkene, photochemical reaction of water.

Unit-5 Photoinduced electron transfer (1+10+1 h)

5.1 Electron transfer (ET)–photoinduced ET in chromophore–quencher, MLCT-ET schemes for type-1 and type-2 metal organic dyads.

5.2 Thermodynamics of photoinduced electron transfer: electron transfer theory, experimental determination of rates of photo induced intramolecular electron transfer, $[Ru(bpy)_3]^{2+}$, Marcus free energy relationship.

5.3 Electrochemistry and photophysics of monoquat(*N*-methyl-4,4'-bipyridine) to $[Ru(bpy)_3]^{2+}$ chromophore. Inner sphere acceptors and donors of bpy ligands, aromatic amine, electro donors, driving force dependence for ET, phenothiazine electron donor, pyrazole and polypyridine.

Text Books

1. Drago, R. S. PhysicaI Methods in Chemistry; Saunders: Philadelphia, 1977.
2. Huheey, J. E.; Keiter, E. A.; Keiter, R. L. *Inorganic Chemistry*; 4th ed.; Harper and Row: New York; 1983.
3. Cotton, F. A.; Wilkinson. G.; Murillo, C. A.; Bochmann, M. *Advanced Inorganic Chemistry*, 6th ed.; Wiley Inter science: NewYork; 1988.
4. Purcell, K. F.; Kotz, J. C. *Inorganic Chemistry*; Saunders: Philadelphia, 1976.
5. Lever. A. B. P. *Inorganic Electronic Spectroscopy*, 2nd Ed.; Elsevier Publishing Company: Amsterdam; 1984.
6. Weil, J. A.; Bolton, J. R.; Wertz, J. E. *Electron Paramagnetic Resonance*; Wiley Interscience; 1994.
7. Bancroft. G. M, *Mossbauer spectroscopy, an introduction for inorganic chemists and geochemists*, McGraw-Hill, London, 1973.
8. Kissinger, P. T.; Heinnan, W. R. *Laboratory Techniques in Electroanalytical Chemistry*; 2nd ed.; Marcel Dekker Inc.: New York; 1996.
9. Sawyer, D. T.; Sobkowiak, A.; Roberts, Jr., J. L. *Electrochemistry for Chemists*, 2nd ed.; Wiley Interscience: New York; 1995.
10. R. Eldik and G. Stochel. *Inorganic Photochemistry*. 2nd ed, Academic Press, 2003.
11. G. J. Ferraudi, *Elements of inorganic photochemistry*, 1st ed, wiley Inter Science, 1988.
12. K. K. Rohatgi Mukherjee, *Fundamentals of photochemistry*, Wiley Eastern Ltd., 1996.

References

1. V. Ramamurthy and K. S. Schanze, *Organic and inorganic photochemistry*, New York, Marcel Dekker, 1998.
2. D. C. Neckers, G. V. Bunav, W. S. Jenks, *Advances in*

Photochemistry, vol. 27, John Wiley & sons, 2002.

3. Parker, D.; Dickins, R. S.; Puschmann, H.; Crossland, C.; Howard, J. A. K. "*Being Excited by Lanthanide Coordination Complexes: Aqua Species, Chirality, Excited-State Chemistry, and Exchange Dynamics*", *Chem. Rev*. **2002**, *102*, 1977-2010.

16PCH3TP01 SUMMER TRAINING PROGRAMME

SEMESTER	**III**	**CREDITS**	**5**
CATEGORY	**TP(P)**	**NO.OF HOURS/ WEEK**	**4**

Objectives:

1. A staff member of a department (GUIDE) will be monitoring the performance of the candidate.
2. The summer training program falls between Semester II and III. Students are expected to undergo this training soon after the second semester examinations.
3. The training will commence not later than one week after the completion of the semester examination
4. Organizations for the summer placement must be confirmed before the commencement of the second continuous internal tests.
5. Students must submit letter of induction to the respective guide within the first week of the internship.
6. The student has to spend a total of 20 working days in the respective field.
7. Students are expected to submit weekly reports along with daily time sheets to the respective supervisors.
8. The reports will be used to evaluate the student's performance.
9. Students should submit a letter of completion from the organization duly signed by the authorities.
10. If the staff is satisfied with the performance of student, he/she will be marked **"COMPLETED"** at the end of the semester and the details will be submitted to COE office through the HOD

16PCH3ID01 MATERIALS SCIENCE

SEMESTER	**III**	**CREDITS**	**5**
CATEGORY	**ID(T)**	**NO.OF HOURS/ WEEK**	**6**

Objectives:

1. To introduce and give an insight into the fascinating area of solid state physics, solid state chemistry and material science.
2. This will enable the students in pursuing higher studies and go for research.

Unit 1: Crystallography (1+23+1 h)

1.1 Introduction - Crystal planes and directions – Unit cells, Miller indices, Two and three dimensional space lattices, crystal systems, reciprocal lattices, symmetry elements (2D &3D), matrix representation of symmetry operations, point groups (2D & 3D) operators - proper and improper axis, mirror planes, Glide planes, screw axis, derivation of space groups (2D and 3D).

1.2 Crystal structure – Analysis by powder X-ray diffraction and single crystal analysis, single crystal analysis and its applications. Electron charge density maps, neutron diffraction – method and applications.

1.3 Growth methods - Kinds of nucleation - equilibrium stability and metastable state-classical theory of nucleation. Single crystal growth – Low and high temperature, solution growth technique – Gel and sol-gel methods. Melt growth - Bridgeman-Stockbarger method, Czochralski method. Flux technique, physical and chemical vapour transport methods.

1.4 Characterization techniques – TG, DTA and DSC methods, SEM and TEM Analysis -working principle and instrumentation. Determination of hardness, elastic behavior - Atomic model of elastic behavior. Modulus as parameter in design rubber like elasticity. Plastic deformation–tensile stress – strain curve. Deformation by slip. Work hardening and dynamic recovery - Effect of grain size and dislocation motion.

Unit 2: Properties of crystals - Optical, dielectric and diffusion studies (1+18+1 h)

2.1 Optical studies - Electromagnetic spectrum (qualitative) – refractive index – reflectance – transparency, translucency and opacity. Types of luminescence – photoluminescence, cathodoluminescence and electroluminescence.

2.2 Dielectric studies- Polarisation - electronic, ionic, orientation, and space charge polarisation. Effect of temperature on dielectric constant. Dielectric loss. Types of dielectric breakdown – intrinsic, thermal, discharge, electrochemical and defect breakdown.

2.3 Diffusion studies - Mechanisms, vacancy and interstitial diffusion – Steady state diffusion–Non-steady state diffusion – Factors influencing diffusion – Diffusing species and temperature – Diffusion in ionic and polymeric materials.

Unit 3: Special Materials (1+13+1 h)

3.1 Semiconductors - Types of semiconductors - intrinsic and extrinsic, direct and indirect band gap, Elemental and compound semiconductors.Defect semiconductors- stoichiometric and non-stoichiometric defects. Applications: p-n junction as transistors and rectifiers, photovoltaic and photogalvanic cell, photoelectrocatalytic splitting of water using TiO_2, $SrTiO_3$, ZnO, $TiO_{2-x}F_x$ and $WO_{3-x}F_x$.

3.2 Superconductivity: Meissner effect, Critical temperature and critical magnetic Field, Type I and Type II superconductors, BCS theory of superconductivity - Cooper pair of electrons, Applications of superconductors.

3.3 Soft and hard magnets - Domain theory - Hysteresis Loop - Applications. Magneto resistance and giant magneto resistance (GMR) materials. Ferro, ferri and antiferromagnetic materials - examples and applications, magnetic parameters for recording applications.

3.4 Ferroelectric, Piezoelecric, and pyroelectric materials – properties and applications. Shape memory Alloys - characteristics and applications, Non- linear optics - Second Harmonic Generators (SHG) , mixing of Laser wave lengths by quartz, ruby and $LiNbO_3$.

Unit 4: Polymers (1+13+1 h)

4.1 Introduction - Monomers, Oligomers, Polymers and their characteristics. Plastics, elastomers, fibres, homopolymers and co-polymers. Bonding in polymers: Primary and secondary bond forces in polymers; cohesive energy. Determination of Molecular mass of polymers: Number Average molecular mass (M_n) and Weight average molecular mass (M_w) of polymers.

4.2 Mechanism and techniques of Polymerization - Chain growth polymerization: Cationic, anionic, free radical polymerization, Stereo regular polymers: Ziegler Natta polymerization, Step growth polymerisation, Bulk, Solution, Emulsion, Suspension, interfacial and gas phase polymerization. Kinetics of polymerization, polymer degradation.

4.3 Reactions of polymers – Hydrolysis, acidolysis, aminolysis, addition and substitution reactions.

4.4 Conducting Polymers: Polyphenylene, polypyrrole and polyacetylene.

4.5 Polymer Processing Techniques - Calendaring, die casting, compression moulding, injection moulding, blow moulding and reinforcing.

Unit 5: Nanomaterials (1+13+1 h)

5.1 Synthesis - Physical and chemical methods - inert gas condensation, arc discharge, laser ablation, sol-gel method, solvothermal and hydrothermal method, chemical vapor deposition (CVD) - reaction types, different kinds of CVD techniques - metallo organic CVD (MOCVD), plasma enhanced CVD (PECVD), and low pressure CVD (LPCVD).

5.2 Classification of nanomaterials - Nanoparticles and nanocomposites - types of nanoparticles, Pure metals - gold and silver. Metal Oxides - silica, iron oxide and alumina. Synthesis and Properties. Core-shell nanoparticles - types, synthesis, and properties. Nanocomposites - metal-matrix, ceramic matrix and polymer-matrix composites - examples and applications.

5.3 Surface characterization - AFM and STM (principle, instrumentation and applications).

5.4 Applications – Nanomaterials for environmental remediation – nanomaterials as sorbents, nanofiltration, and nanoscale biopolymers and nanoreactors for remediation.

Books for study

1. James F. Shackelford and Madanapalli K. Muralidhara, Introduction to Materials Science for Engineers. 6th ed., PEARSON Press, 2007.
2. P.K. Palanisamy, Materials Science, Scitech Publications, India, 2002.
3. T. Balachandran, Materials Science, Charulatha Publications, India, 2003.
4. V. R. Gowariker, *Polymer Science*, Wiley Eastern, 1995.
5. G. S. Misra, *Introductory Polymer Chemistry*, New Age International (Pvt) Limited, 1996.
6. Fred W Billmeyer, Textbook of Polymer Science, John Wiley & sons, 1984.
7. Charles P. Poole, Jr., Frank J. Owens, Introduction to nanotechnology, Wiley-India, 2009.
8. T. Pradeep, Nano: The Essentials, Tata McGraw-Hill Publishing Company Limited, 2007.
9. T. Pradeep, A Text book of nanoscience and nanotechnology, Tata Mc-Graw-Hill, New Delhi, 2012.

Books for reference:

1. M.G. Arora, Solid State Chemistry, Anmol Publications, New Delhi, 2001.
2. R.K. Puri and V. K. Babbar, Solid State Physics, Schad and Company Ltd, 2001.
3. C. Kittel, Solid State Physics, John-Wiley and sons, NY, 1966.
4. H.P. Meyers, Introductory Solid State Physics, Viva Books Private Limited, 1998.
5. A.R. West, solid State Chemistry and Applications, John-Wiley and sons, 1987.
6. R. J. Young, P. A. Lovell, *Introduction to Polymers*, Technology & Engineering, 2011.
7. B. Viswanathan, Nanomaterials, Narosa Publishing House Pvt. Ltd., New Delhi, 2009.
8. Sulabha K. Kulkarni, Nanotechnology - Principles and Practices, Capital Publishing Company, New Delhi, 2007.
9. S. Shanmugam, Nanotechnology, MJP Publishers, Chennai, 2010.
10. P. M. Sivakumar, V. I. Kodolov, G. E. Zaikov, A. K. Haghi, *Nanostructure, Nanosystems, and Nanostructured Materials: Theory - Production and Development,*Technology & Engineering, 2013.

16PCH4MC01 ORGANIC SYNTHESIS AND PHOTOCHEMISTRY

SEMESTER	**IV**	**CREDITS**	**4**
CATEGORY	**MC(T)**	**NO.OF HOURS/ WEEK**	**5**

Objectives

1. To understand the molecular complexity of carbon skeletons and the presence of functional groups and their relative positions.
2. To apply disconnection approach and identifying suitable synthon to effect successful organic synthesis.

3. To study various synthetically important reagents for any successful organic synthesis
4. To learn the concepts of pericyclic reaction mechanisms.
5. To gain the knowledge of photochemical organic reactions.

Unit 1: Reagents for Organic Synthesis (1+16+1 h)

1.1 Reagents for functional group transformations: Lithium diisopropylamide (LDA), Gilmann reagent, dicyclohexylcarbodimide (DCC), dichlorodicyanoquinone (DDQ), Silane reagents-trialkylsilyl halides, trimethylsilyl cyanide, trimethylsilane, t-butyldimethylsilane.

1.2 Crown ethers, cyclodextrins, Ziegler-Natta catalyst, diazomethane, Stark enamine reaction, phosphorous ylides- Wittig and related reactions, sulphur ylides–reactions with aldehydes and ketones, 1,3-dithiane anions, Peterson reaction.

Unit 2: Modern Synthetic Reactions (1+21+1 h)

2.1 Chromium and manganese reagents (PCC, PDC, Jones reagent, MnO_2), Oxygen (singlet and triplet), ozone, peroxides and peracids, lead tetraacetate, periodic acid, NBS, chloramine-T, Sommelet oxidation, Oppenauer oxidation, Fenton's reagent, Sharpless asymmetric epoxidation.

2.2 Catalytic hydrogenation (homogeneous and heterogeneous) – catalysts (Pt, Pd, Rh-C, Ni, Ru), Wilkinson catalyst, $LiAlH_4$ and derivatives of LAH, $NaBH_4$, DIBAL-H, Sodium cyanoborohydride, dissolving metal reactions (Birch reduction). Leukart reaction (reductive amination) Diborane as reducing agent, Meerwein-Ponndorf-Verley reduction, tributyltin hydride, stannous chloride, and Baker's yeast reduction.

2.3 Named Reactions: Suzuki coupling, Heck reaction, Negishi reaction. Baylis-Hillman reaction, Henry reaction Nef reaction, Kulikovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction, Ugi reaction. Brook rearrangement: Tebbe olefination, metal mediated C-C and C-X coupling reactions: Stille, Sonogashira, Nozaki Hiyama, Buchwald - Hartwig, Ullmann coupling reactions, directed orthometalation.

2.4 Electroorganic synthesis: Electro-oxidation and -reduction reactions.

Unit 3: Organic Synthetic Methodology (1+16+1 h)

3.1 Retrosynthetic analysis; Alternate synthetic routes. Synthesis of organic mono and bifunctional compounds via disconnection approach. Key intermediates, available starting materials and resulting yields of alternative methods.

3.2 Convergent and divergent synthesis, Synthesis based on umpolung concepts of seebach. Protection of hydroxyl, carboxyl, carbonyl, thiol and amino groups. Illustration of protection and deprotection in synthesis.

3.3 Control elements: Regiospecific control elements. Use of protective groups, activating groups, and bridging elements. Stereospecific control elements. Functional group alterations and transposition.

Unit 4: Pericyclic Reactions (1+12+1 h)

4.1 Woodward Hoffmann rules; The Mobius and Huckel concept, FMO method and correlation diagrams.

4.2 Cycloaddition and Cheletropic reactions; [2+2], [2+4], [6+4] and 1,3-dipolar cycloadditions; Electrocyclization reactions of conjugated dienes and trienes. Sigmatropic rearrangements: (1,3), (1,5), (3,3) and (5,5)-carbon migrations, degenerate rearrangements. Group transfer reactions.

Unit 5: Organic Photochemistry (1+15+1 h)

5.1 Photochemical excitation: Experimental techniques; electronic transitions; Jablonskii diagrams; intersystem crossings; energy transfer processes; Stern Volmer equation.

5.2 Reactions of electronically excited ketones; $\pi \rightarrow \pi^*$ triplets; Norrish type-I and type-II cleavage reactions; photo reductions; Paterno-Buchi reactions; photochemistry of α,β-unsaturated ketones; cis-trans isomerisation.

5.3 Photon energy transfer reactions, Photocycloadditions, Photochemistry of aromatic compounds; photochemical rearrangements; photostationery state; di-π-methane rearrangement; Reaction of conjugated cyclohexadienone to 3,4-diphenyl phenols; Barton's reactions; Low temperature photochemistry, Flash photolysis.

Text Books

1. F. A. Carey and Sundberg, *Advanced Organic Chemistry, 5th ed*, Tata McGraw-Hill, New York, 2003.
2. J. March and M. Smith, *Advanced Organic Chemistry*, 5th ed., John-Wiley and sons, 2007.
3. I. Fleming, *Pericyclic Reactions*, Oxford Science Publications, Cambridge, 1999.
4. R. E. Ireland, *Organic synthesis*, Prentice Hall India, Goel publishing house, 1990.
5. M. B. Smith, *Organic synthesis*, McGraw Hill International Edition 1994.
6. H. O. House. *Modern Synthetic reactions*, W.A. Benjamin Inc, 1972.
7. J. C*layden*, N. Greeves, S. Warren and Wothers, *Organic Chemistry 2nd edn*, Oxford University Press, New York, 2012.

References

1. Gill and Wills, *Pericyclic Reactions*, Chapman Hall, London, 1974.
2. W. Caruthers, *Modern methods of organic synthesis*, Cambridge University Press, 1993.

3. R. O. C. Norman, *Organic synthesis*, Chapman Hall, London, 1980.

16PCH4MC02 ELECTROCHEMISTRY

SEMESTER	**IV**	**CREDITS**	**5**
CATEGORY	**MC(T)**	**NO.OF HOURS/ WEEK**	**6**

Objectives:

1. To understand the behavior of electrolytes in solution.
2. To know the structure of the electrode surface.
3. To understand the importance of electrode kinetics and to know the applications of electrode process.

Unit 1: Ionics (1+21+1 h)

1.1 Arrhenius theory of electrolytic dissociation- limitations, van’t Hoff factor and its relation to colligative properties. Deviation from ideal behavior. Ionic activity, ion solvent and ion-ion interactions. Expression for free energy. Debye-Huckel theory of strong electrolytes. Debye-Huckel length and potential around a central ion, its interpretation. Debye-Huckel-Bjerrum model. Debye-Huckel limiting law –derivation, modifications and applications.

1.2 Electrolytic conduction- Debye-Huckel-Onsager treatment of the conductance of strong electrolyte- experimental verification and limitations. Evidence for the existence of ionic atmosphere. Ion association and triple ion formations. Anomalous conductance of nonaqueous electrolytic solution. Abnormal mobility of hydrogen and hydroxyl ions.

1.3 Evaluation of thermodynamic quantities – ΔG, ΔH and ΔS. Calculation of K_a, K_b, K_{sp}, K_w, K_h and pH using emf data.

Unit 2: Electrical Double Layer (1+10+1 h)

2.1 Interfacial phenomena - Evidences for electrical double layer, polarisable and non-polarisable interfaces. Electrocapillarity - Lipmann's equation, electro capillary curves. Electro-kinetic phenomena electro-osmosis, electrophoresis, streaming and sedimentation potentials, mention of colloidal and poly electrolytes.

2.2 Structure of electrical double layer: Helmholtz-Perrin, Guoy-Chapmann and Stern models of electrical double layer- Applications and limitations.

Unit 3: Electrodics of Elementary Electrode Reactions

(1+15+1 h)

3.1 Behavior of electrodes: Standard electrodes and electrodes at equilibrium. Ohmic and non-Ohmic behaviors. Study of electrode reaction. The model of three electrode system. Sign conventions. Rates of electro chemical reactions. Over potential and chemical & electro chemical conditions for the discharge of ions.

3.2 Rates of simple electrode reactions-elementary electron-electrode process. Butler- Volmer equation- Exchange current density and symmetry factor- experimental determinations- electrode rectification. Nernst equation as a special case of Butler -Volmer equation – Reaction resistance- polarisable& non-polarisable electrodes- Low and high field approximations-Tafel equations.

Unit 4: Electrodics of Multistep Multi Electron System

(1+16+1 h)

4.1 Rates of multi-step electrode reactions, Butler - Volmer equation for a multi-step reaction (examples of multi electron reactions). Rate determining step of an electrode reaction. Transfer coefficients and stoichiometric number.

4.2 Electro-chemical reaction mechanisms Proposal of electro-chemical reaction mechanisms- Electrochemical reaction order. Surface coverage - Rate expressions. Reduction of (i) I_3^- and (ii) Fe^{2+}. Dissolution of iron to iron (II). Overvoltage and evolution of oxygen and hydrogen at different pH. Symmetry factors vs transfer coefficients. Corrosion and passivation of metals-Pourbiax and Evan’s diagrams.

Unit 5: Concentration Polarisation and Electroanalytical Techniques (1+18+1 h)

5.1 Transport of the electro active species to electrode- Different types of over voltages-Chemical and electro chemical over potentials. Phase, activation and concentration over potentials.

5.2 Diffusion, migration and hydrodynamic modes of transports. The role of supporting electrolytes. Polarography- principle and applications, principle of square wave polarography, cyclic voltammetry-, anodic and cathodic stripping voltammetry, differential pulse voltammetry and amperometric titrations.

5.3 Electrochemical process as source of energy – sodium and lithium ion batteries, solid oxide fuel cells, electrocatalysis – anodically and cathodically initiated processes.

Text Books

1. D. R. Crow, *Principles and applications of electrochemistry*, 4th edition, Chapman & Hall/CRC, 2014.

2. J. Rajaram and J.C. Kuriakose, "*Kinetics and Mechanism of chemical Transformations*", Macmillan India Ltd., New Delhi, 2011.
3. S. Glasstone, *Electro chemistry*, Affiliated East-West Press, Pvt., Ltd., New Delhi, 2008.
4. B. Viswanathan, S. Sundaram, R. Venkataraman, K. Rengarajan and P.S. Raghavan, *Electrochemistry-Principles and applications*, S. Viswanathan Printers, Chennai, 2007.
5. Joseph Wang, *Analytical Electrochemistry*, 2nd edition, Wiley, 2004.

References

1. J.O.M.Bockris and A.K.N.Reddy, *Modern Electro chemistry*, vol.1 and 2B, Springer, Plenum Press, New York, 2008.
2. J.O.M.Bockris, A.K.N.Reddy and M.G. Aldeco *Morden Electro chemistry*, vol. 2A, Springer, Plenum Press , New York, 2008.
3. Philip H. Rieger, *Electrochemistry*, 2nd edition, Springer, New York, 2010.
4. L.I.Antropov, *Theoretical electrochemistry*, Mir Publishers, 1977.
5. K.L.Kapoor, *A Text book of Physical chemistry*, volume-3, Macmillan, 2001.

16PCH4MC03 PHYSICAL CHEMISTRY PRACTICAL – II

SEMESTER	**IV**	**CREDITS**	**3**
CATEGORY	**MC(L)**	**NO.OF HOURS/ WEEK**	**4**

Objectives

1. To understand and apply the concepts of electrochemistry.

2. To learn sample handling in different experimental techniques.
3. To learn the operations of instrumentals techniques for quantitative estimation.

Experiments

1. Determination of the equivalent conductance at different concentrations and to examine the validity of the Onsager's theory as limiting law at high dilutions for a strong electrolyte.
2. Verification of Ostwald's dilution Law and determination of dissociation constant of weak acid or weak base.
3. Condutometric titration of mixture of strong and weak acids with a strong base.
4. Comparing the relative strengths of acetic and monochloro acetic acid by conductance method.
5. Determination of solubility product of inorganic compounds using conductometer.
6. Determination of the strength of Fe (II) by potentiometric redox titration.
7. Determination of the amount of KCl and KI present in a mixture by potentiometric titration.
8. Determination of pK_{a1} and pK_{a2} of a weak dibasic acid by potentiometry.
9. Determination of dissociation constant of weak acid by potentiometry.
10. Calibration of a pH meter and measurement of pH of different buffer solutions.
11. Determination of pH of the given solution with the help of indicators using buffer solutions and by colorimetric method.
12. Determination of metal to ligand ratio of complexes by Job's method using UV-visible Spectrophotometer.
13. Determination of functional groups using FT-IR spectrometer.

14. Determination of the concentration of a given solution by studying the reversibility of a redox process by Cyclic voltammetry.
15. Estimation of iron, copper and nickel by spectrophotometric method.
16. Separation and analysis of mixtures using HPLC.

Text Books

1. B. Viswanathan and P.S. Raghavan, Practical Physical Chemistry, Viva Books, New Delhi, 2009.
2. Sundaram, Krishnan, Raghavan, Practical Chemistry (Part II), S. Viswanathan Co. Pvt., 1996.

References

1. J. B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.
2. G. W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th edition, McGraw Hill, 2009.
3. J. N. Gurthu and R. Kapoor, Advanced Experimental Chemistry, S. Chand and Co., 1987.

16PCH4PJ01 DISSERTATION/PROJECT

SEMESTER	**IV**	**CREDITS**	**12**
CATEGORY	**MC(PJ)**	**NO.OF HOURS/ WEEK**	**15**

Objectives

To make the student to understand and present a research finding on a topic in the subject related to Chemistry under the guidance of a department staff.

Testing

The student will be tested both in subject matter of the report and the mode of presentation in a review meeting to be held in the middle of the semester, with a panel of three senior staff of the department. This progress reporting will carry 20% marks. Upon submission of the project report to the office of the Controller of Examinations, the viva-voce examination will be conducted by the supervisor and the external expert suggested by the supervisor. The project report and the viva-voce will be evaluated for 80% marks.

Project report: **60 Marks**

Standard of subject and plan

Preparation and mastery

Originality and logical development

Summary and references

Viva-voce **20 Marks**

Economy of time

Communication

Blackboard use and teaching aids

Language and diction

Answer to questions