BRANCH IVB

M. Sc.
POLYMER CHEMISTRY

FOREWORD

I feel highly privileged in presenting the revised curricula and syllabi of Branch IVB M.Sc. Polymer Chemistry for favour of approval by the Faculty and Academic Council of the University.

As per Mahatma Gandhi University PG Programme Regulations for Credit Semester System 2011(MGU-CSS-PG) it has been decided to introduce the Credit Semester System for all the PG courses which are being offered by the affiliated colleges/institutions of the University with effect from the academic year 2012-2013 admission onwards. The PG Board of Studies in Chemistry was entrusted with the duty of preparing the revised curricula and syllabi for all the five M.Sc. Programmes in Chemistry currently approved by the University and offered in the affiliated colleges.

The BOS prepared draft proposals of revised curricula and syllabi for all the M.Sc. courses in Chemistry in conformity with the broad guidelines issued by the University to suit the Credit Semester System. The draft curricula and syllabi for all the five M.Sc. Programmes were discussed in a very effective manner with active participation of Resource Persons and Teacher Representatives from all the colleges in a three-day workshop. The workshop was a grand success and the BOS could incorporate many of the suggestions while finalizing the proposal of the Restructured Curricula and Syllabi.

The BOS feel that appreciable updating could be done in keeping with the current developments and trends in chemistry education. The task of preparing the Curricula and Syllabi and bringing it out in the present form for all the five M.Sc. courses was not a simple task but it was possible with dedicated efforts and wholehearted support and involvement of all the members of the BOS. I would like to express my sincere thanks to all my fellow members of the BOS for all their whole hearted time-bound help, cooperation and encouragement. It has been a pleasure for me to work with them. I am also thankful to all Resource Persons and Teacher Representatives of the colleges for their active participation and useful suggestions during the three-day workshop.

Prof. (Dr.) P. K. Radhakrishnan
Chairman, PG Board of Studies in Chemistry

PG Board of Studies in Chemistry

1. **Dr. P.K. Radhakrishnan** **(Chairman)**
   Professor, School of Chemical Sciences
   Mahatma Gandhi University
   Kottayam-686560

2. **Dr. S. Sugunan**
   Professor, Department of Applied Chemistry
   CUSAT
   Kochi-682022

3. **Dr. Baby Thomas**
   Associate Professor, Department of Chemistry
   St. Dominic's College
   Kanjirappally-686512

4. **Dr. Varghese Philip**
   Associate Professor, Department of Chemistry
   St. Thomas College
   Kozhenchery-689641

5. **K.C. Joseph**
   Associate Professor, Department of Chemistry
   St. Joseph's College
   Moolamattom-685591

6. **Dr. Sunny Kuriakose**
   Associate Professor, Department of Chemistry
   St. Thomas College
   Pala-686574

7. **Dr. Ibnu Saud**
   Associate Professor, School of Chemical Sciences
   Mahatma Gandhi University
   Kottayam-686560

8. **J.L. Rajan**
   Associate Professor, Department of Chemistry
   KE College
   Mannanam-686561

9. **Dr. K. Sreevalsan**
   Associate Professor, Department of Chemistry
   SN College
   Kollam-691001

	Code	Course	Hours/ Week	Total Hours	Credit
Semester 1	PO1C01	Organometallics and Nuclear Chemistry	4	72	4
	PO1C02	Structural and Molecular Organic Chemistry	4	72	4
	PO1C03	Quantum chemistry and Group Theory	4	72	4
	PO1C04	Classical and Statistical Thermodynamics	3	54	3
	PO2P01	Inorganic Chemistry Practical	3	54	Evaluation at the end of 2nd semester
	PO2P02	Organic Chemistry Practical	3	54	
	PO2P03	Physical Chemistry Practical	4	72	
		Total	**25**	**450**	**15**
Semester 2	PO2C05	Coordination Chemistry	4	72	4
	PO2C06	Organic Reaction Mechanisms	4	72	4
	PO2C07	Chemical Bonding and Computational Chemistry	4	72	4
	PO2C08	Molecular Spectroscopy	3	54	3
	PO2P01	Inorganic Chemistry Practical	3	54	3
	PO2P02	Organic Chemistry Practical	3	54	3
	PO2P03	Physical Chemistry Practical	4	72	3
		Total	**25**	**450**	**24**
Semester 3	PO3C09	Structural Inorganic Chemistry	4	72	4
	PO3C10	Physical Chemistry	4	72	4
	PO3C11	Concepts of Polymer Chemistry	4	72	4
	PO3C12	Spectroscopic Methods in Chemistry	3	54	3
	PO4P04	Polymer Preparative Practical	3	54	Evaluation at the end of 4th semester
	PO4P05	Polymer Characterization Practical	3	54	
	PO4P06	Polymer Processing & Testing Practical	4	72	
		Total	**25**	**450**	**15**
Semester 4		Elective 1	5	90	4
		Elective 2	5	90	4
		Elective 3	5	90	4
	PO4P04	Polymer Preparative Practical		54	3
	PO4P05	Polymer Characterization Practical	3	54	3
	PO4P06	Polymer Processing & Testing Practical	4	72	3
	PO4D01	Project			3
	PO4V01	Viva			2
		Total	**25**	**450**	**26**
Grand Total					**80**

SEMESTER 1

PO1C01 ORGANOMETALLICS AND NUCLEAR CHEMISTRY

Credit: 4 **Contact Lecture Hours: 72**

Unit 1: Organometallic Compounds- Synthesis, Structure and Bonding (18 Hours)

1.1 Organometallic compounds with linear pi donor ligands-olefins, acetylenes, dienes and allyl complexes-synthesis, structure and bonding.

1.2 Complexes with cyclic pi donors-metallocenes and cyclic arene complexes-structure and bonding. Hapto nomenclature. Carbene and carbyne complexes.

1.3 Preparation, properties, structure and bonding of simple mono and binuclear metal carbonyls, metal nitrosyls, metal cyanides and dinitrogen complexes. Polynuclear metal carbonyls with and without bridging. Carbonyl clusters-LNCCS and HNCCS, Isoelectronic and isolobal analogy, Wade-Mingos rules, cluster valence electrons.

Unit 2: Reactions of Organometallic Compounds (9 Hrs)

2.1 Substitution reactions-nucleophilic ligand substitution, nucleophilic and electrophilic attack on coordinated ligands.

2.2 Addition and elimination reactions-1,2 additions to double bonds, carbonylation and decarbonylation, oxidative addition and reductive elimination, insertion (migration) and elimination reactions.

2.3 Rearrangement reactions, redistribution reactions, fluxional isomerism.

Unit 3: Catalysis by Organometallic Compounds (9 Hrs)

3.1 Homogeneous and heterogeneous organometallic catalysis-alkene hydrogenation using Wilkinson catalyst, Tolman catalytic loops.

3.2 Reactions of carbon monoxide and hydrogen-the water gas shift reaction, the Fischer-Tropsch reaction(synthesis of gasoline).

3.3 Hydroformylation of olefins using cobalt or rhodium catalyst.

3.4 Polymerization by organometallic initiators and templates for chain propagation-Ziegler Natta catalysts.

3.5 Carbonylation reactions-Monsanto acetic acid process, carbonylation of butadiene using $Co_2(CO)_8$ catalyst in adipic ester synthesis.

3.6 Olefin methathesis-synthesis gas based reactions, photodehydrogenation catalyst ("Platinum Pop"). Palladium catalysed oxidation of ethylene-the Wacker process.

Unit 4: Organometallic Polymers **(9 Hrs)**

4.1 Polymers with organometallic moieties as pendant groups, polymers with organometallic moieties in the main chain, condensation polymers based on ferrocene and on rigid rod polyynes, polymers prepared by ring opening polymerization, organometallic dendrimers.

Unit 5: Bioinorganic Compounds **(18 Hrs)**

5.1 Essential and trace elements in biological systems, structure and functions of biological membranes, mechanism of ion transport across membranes, sodium pump, ionophores, valinomycin and crown ether complexes of Na^+ and K^+, ATP and ADP. Photosynthesis-chlorophyll a, PS I and PS II. Role of calcium in muscle contraction, blood clotting mechanism and biological calcification.

5.2 Oxygen carriers and oxygen transport proteins-haemoglobins, myoglobins and haemocyanin, haemerythrins and haemevanadins, cooperativity in haemoglobin. Iron storage and transport in biological systems-ferritin and transferrin. Redox metalloenzymes-cytochromes, peroxidases and superoxide dismutase and catalases. Nonredox metalloenzymes-CarboxypeptidaseA-structure and functions. Nitrogen Fixation-nitrogenase, vitamin B_{12} and the vitamin B_{12} coenzymes.

5.3 Metals in medicine-therapeutic applications of *cis*-platin, radio-isotopes and MRI agents. Toxic effects of metals(Cd, Hg, Cr and Pb).

Unit 6: Nuclear Chemistry **(9 Hrs)**

6.1 Fission products and fission yield. Neutron capture cross section and critical size. Nuclear fusion reactions and their applications. Chemical effects of nuclear transformations. Positron annihilation and autoradiography. Principles of counting technique such as G.M. counter, proportional, ionization and scintillation counters. Cloud chamber.

6.2 Synthesis of transuranic elements such as Neptunium, Plutonium, Curium, Berkelium, Einsteinium, Mendelevium, Nobelium, Lawrencium and elements with atomic numbers 104 to 109.

6.3 Analytical applications of radioisotopes-radiometric titrations, kinetics of exchange reactions, measurement of physical constants including diffusion constants, Radioanalysis, Neutron Activation Analysis, Prompt Gama Neutron Activation Analysis and Neutron Absorptiometry.

6.4 Applications of radio isotopes in industry, medicine, autoradiography, radiopharmacology, radiation safety precaution, nuclear waste disposal. Radiation chemistry of water and aqueous solutions.

6.5. Measurement of radiation doses. Relevance of radiation chemistry in biology, organic compounds and radiation polymerization.

References

01. J.E. Huheey, E.A. Keiter, R.L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Harper Collins College Publishers,1993.

02. F.A. Cotton, G. Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th edition, Wiley-Interscience, 1999.

03. K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.

04. P. Powell, Principles of Organometallic Chemistry, 2nd Edn., Chapman and Hall, 1988.

05. B.E. Douglas, D.H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007.

06. B.D. Guptha, A.J Elias, Basic Organometallic Chemistry, Universities Press, 2010.

07. R.W. Hay, Bio Inorganic Chemistry, Ellis Horwood, 1984.

08. H.J. Arnikar, Essentials of Nuclear Chemistry, Wiley Eastern, 1982.

09. S.N. Goshal, Nuclear Physics, S. Chand and Company, 2006.

PO1C02 STRUCTURAL AND MOLECULAR ORGANIC CHEMISTRY

Credit: 4 **Contact Lecture Hours: 72**

Unit 1: Basic Concepts in Organic Chemistry (18 Hrs)

1.1 Review of basic concepts in organic chemistry: bonding, hybridisation, MO picture, inductive effect, electromeric effect, resonance effect, hyperconjugation, steric effect. Bonding weaker than covalent bonds.

1.2 The formalism of curved arrow mechanisms. Practicing of line diagram drawing.

1.3 Concept of aromaticity: delocalization of electrons - Hückel's rule, criteria for aromaticity, examples of neutral and charged aromatic systems - annulenes. NMR as a tool for aromaticity. Anti-and homo-aromatic systems - Fullerenes, Carbon nanotubes and Graphene.

1.4 Mechanism of electrophilic and nucleophilic aromatic substitution reactions with examples. Arenium ion intermediates. SN1, SNAr, SRN1 and Benzyne mechanisms.

Unit 2: Physical Organic Chemistry and Photochemistry (18 Hrs)

2.1 Energy profiles. Kinetic versus thermodynamic control of product formation,Hammond postulate, kinetic isotope effects with examples, Hammet equation, Taft equation. Linear free energy relationships.

2.2 Catalysis by acids and bases and nucleophiles with examples from acetal, cyanhydrin and ester formation and hydrolysis reactions-AAC2, AAC1, AAL1, BAC2and BAL1 mechanisms. Solvent effect. Bulk and specific solvent effects. Introduction to carbon acids - pKa of weak acids, kinetic and thermodynamic acidity. Hard and soft acids and bases - HSAB principle and its applications.

2.3 Photoreactions of carbonyl compounds: Norrish reactions of ketones. Patterno-Buchi reaction. Barton, Di-π-methane and photo Fries rearrangements. Photochemistry of nitro and azo groups.

Unit 3: Stereochemistry of Organic Compounds (18 Hrs)

3.1 Introduction to molecular symmetry and chirality: examples from common objects to molecules. Axis, plane, center, alternating axis of symmetry.

3.2 Center of chirality: molecules with C, N, S based chiral centers, absolute configuration, enantiomers, racemic modifications, R and S nomenclature using Cahn-Ingold-Prelog rules, molecules with a chiral center and Cn, molecules with more than one center of chirality, definition of diastereoisomers, constitutionally symmetrical and unsymmetrical chiral molecules, erythro, threo nomenclature.

3.3 Axial, planar and helical chirality with examples, stereochemistry and absolute configuration of allenes, biphenyls and binaphthyls, ansa and cyclophanic compounds, spiranes, exo-cyclic alkylidenecycloalkanes.

3.4 Topicity and prostereoisomerism, topicity of ligands and faces as well as their nomenclature. NMR distinction of enantiotopic/diastereotopic ligands.

3.5 Stereoisomerism: definition based on symmetry and energy criteria, configuration and conformational stereoisomers.

3.6 Geometrical isomerism: nomenclature, E-Z notation, methods of determination of geometrical isomers. Interconversion of geometrical isomers.

Unit 4: Conformational Analysis (18 Hrs)

4.1 Conformational descriptors - factors affecting conformational stability of molecules. Conformational analysis of acyclic and cyclic systems: substituted ethanes, cyclohexane and its derivatives, decalins, adamantane, congressane, sucrose and lactose. Fused and bridged bicyclic systems. Conformation and reactivity of elimination (dehalogenation, dehydrohalogenation, semipinacolic deamination and pyrolytic elimination-Saytzeff and Hofmann eliminations), substitution and oxidation of 2^0 alcohols. Chemical consequence of conformational equilibrium -Curtin Hammett principle.

References

01. R. Bruckner, Advanced Organic Chemistry: Reaction Mechanisms, Academic Press, 2002.

02. F.A. Carey, R.A. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5^{th} Edn., Springer, 2007.

03. J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2004.

04. T.H. Lowry, K.S. Richardson, Mechanism and Theory in Organic Chemistry, 2^{nd} Edn., Harper & Row, 1981.

05. N.S. Isaacs, Physical Organic Chemistry, ELBS/Longman, 1987.

06. D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, 3^{rd} Edn., New Age Pub., 2010.

07. D.G. Morris, Stereochemistry, RSC, 2001.

08. E.L. Eliel, S.H. Wilen, Stereochemistry of Organic Compounds, John Wiley & Sons, 1994.

09. N.J. Turro, V. Ramamurthy, J.C. Scaiano, Principles of Molecular Photochemistry: An Introduction, University Science books, 2009.

10. N.J. Turro, Modern Molecular Photochemistry, Benjamin Cummings, 1978.

11. K.K.R. Mukherjee, Fundamentals of Photochemistry, New Age Pub., 1978.

PO1C03 QUANTUM CHEMISTRY AND GROUP THEORY

Credit: 4 **Contact Lecture Hours: 72**

Unit 1: Postulates of Quantum Mechanics **(9 Hrs)**

1.1 State function or wave function postulate: Born interpretation of the wave function, well behaved functions, orthonormality of wave functions.

1.2 Operator postulate: operator algebra, linear and nonlinear operators, Laplacian operator, commuting and noncommuting operators, Hermitian operators and their properties, eigen functions and eigen values of an operator.

1.3 Eigen value postulate: eigen value equation, eigen functions of commuting operators.

1.4 Expectation value postulate.

1.5 Postulate of time-dependent Schrödinger equation, conservative systems and time-independent Schrödinger equation.

Unit 2: Application to Exactly Solvable Model Problems **(18 Hrs)**

2.1 Translational motion: free particle in one-dimension, particle in a one-dimensional box with infinite potential walls, particle in a one-dimensional box with finite potential walls-tunneling, particle in a three dimensional box-separation of variables, degeneracy.

2.2 Vibrational motion: one-dimensional harmonic oscillator (complete treatment), Hermite equation(solving by method of power series), Hermite polynomials, recursion relation, wave functions and energies-important features, Harmonic oscillator model and molecular vibrations.

2.3 Rotational motion: co-ordinate systems, cartesian, cylindrical polar and spherical polar coordinates and their relationships. The wave equation in spherical polar coordinates-particle on a ring, the phi equation and its solution, wave functions in the real form. Non-planar rigid rotor (or particle on a sphere)-separation of variables, the phi and the theta equations and their solutions, Legendre and associated Legendre equations, Legendre and associated Legendre polynomials. Spherical harmonics (imaginary and real forms)-polar diagrams of spherical harmonics.

2.4 Quantization of angular momentum, quantum mechanical operators corresponding to angular momenta (L_x, L_y, L_z and L^2)-commutation relations between these operators. Spherical harmonics as eigen functions of angular momentum operators L_z and L^2. Ladder operator method for angular momentum. Space quantization.

Unit 3: Quantum Mechanics of Hydrogen-like Atoms **(9 Hrs)**

3.1 Potential energy of hydrogen-like systems. The wave equation in spherical polar coordinates: separation of variables-R, theta and phi equations and their solutions, wave functions and energies of hydrogen-like atoms. Orbitals-radial functions, radial distribution functions, angular functions and their plots.

3.2 The postulate of spin by Uhlenbeck and Goudsmith, discovery of spin-Stern Gerlach experiment. Spin orbitals-construction of spin orbitals from orbitals and spin functions.

Unit 4: Symmetry and Groups **(9 Hrs)**

4.1 Symmetry elements, symmetry operations, point groups and their symbols, sub groups, classes, abelian and cyclic groups, group multiplication tables-classes in a group and similarity transformation.

4.2 Symmetry in crystals-32 crystallographic point groups (no derivation), Hermann-Mauguin symbols. Screw axis-pitch and fold of screw axis. Glide planes. Space groups-determination of space group symbols of triclinic and monoclinic systems.

Unit 5: Theory of Molecular Symmetry **(18 Hrs)**

5.1 Matrices: addition and multiplication of matrices, inverse and orthogonal matrices, character of a matrix, block diagonalisation, matrix representation of symmetry operations, representation of groups by matrices, construction of representation using vectors and atomic orbitals as basis, representation generated by cartesian coordinates positioned on the atoms of a molecule (H_2O and SO_2 as examples).

5.2 Reducible and irreducible representations-construction of irreducible representation by standard reduction formula. Statement of Great Orthogonality Theorem (GOT). Properties of irreducible representations. Construction of irreducible representation using GOT-construction of character tables for C_{2v}, C_{2h}, C_{3v} and C_{4v}. Direct product of representations.

5.3 Molecular dissymmetry and optical activity.

Unit 6: Application of Group Theory in Spectroscopy **(9 Hrs)**

6.1 Applications in vibrational spectra: transition moment integral, vanishing of integrals, symmetry aspects of molecular vibrations, vibrations of polyatomic molecules-selection rules for vibrational absorption. Determination of the symmetry of normal modes of H_2O, Trans N_2F_2 and NH_3 using Cartesian coordinates and internal coordinates. Complementary character of IR and Raman spectra-determination of the number of active IR and Raman lines.

6.2 Application in electronic spectra: selection rules for electronic transition, electronic transitions due to the carbonyl chromophore in formaldehyde.

References

01. I.N. Levine, Quantum Chemistry, 6th Edn., Pearson Education Inc., 2009.
02. P.W. Atkins, R.S. Friedman, Molecular Quantum Mechanics, 4th Edn., Oxford University Press, 2005.
03. D.A. McQuarrie, Quantum Chemistry, University Science Books, 2008.
04. J.P. Lowe, K Peterson, Quantum Chemistry, 3rd Edn., Academic Press, 2006.
05. R. Anatharaman, Fundamentals of Quantum Chemistry, Macmillan India, 2001.
06. R.K. Prasad, Quantum Chemistry, 3rd Edn., New Age International, 2006.
07. T. Engel, Quantum Chemistry and Spectroscopy, Pearson Education, 2006.
08. H. Metiu, Physical Chemistry: Quantum Mechanics, Taylor & Francis, 2006.
09. L. Pauling, E.B. Wilson, Introduction to Quantum Mechanics, McGraw-Hill, 1935.
10. M.S. Pathania, Quantum Chemistry and Spectroscopy (Problems & Solutions), Vishal Publications, 1984.
11. F.A. Cotton, Chemical Applications of Group Theory, 3rd Edn., Wiley Eastern, 1990.
12. L. H. Hall, Group Theory and Symmetry in Chemistry, McGraw Hill,1969
13. V. Ramakrishnan, M.S. Gopinathan, Group Theory in Chemistry, Vishal Publications, 1992.
14. S. Swarnalakshmi, T. Saroja, R.M. Ezhilarasi, A Simple Approach to Group Theory in Chemistry, Universities Press, 2008.
15. S.F.A. Kettle, Symmetry and Structure: Readable Group Theory for Chemists, 3rd Edn**.,** Wiley, 2007.
16. A. Vincent, Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications, 2nd Edn., Wiley, 2000.
17. A. S. Kunju, G. Krishnan, Group Theory and its Applications in Chemistry, PHI Learning, 2010

PO1C04 CLASSICAL AND STATISTICAL THERMODYNAMICS

Credit: 3 **Contact Lecture Hours- 54**

Unit 1: Classical Thermodynamics **(27 Hrs)**

1.01 Entropy, dependence of entropy on variables of a system (S,T and V; S,T and P). Thermodynamic equations of state. Irreversible processes - Clausius inequality.

1.02 Free energy, Maxwell relations and significance, temperature dependence of free energy - Gibbs Helmholtz equation, applications of Gibbs Helmholtz equation.

1.03 Partial molar quantities, chemical potential and Gibbs-Duhem equations, determination of partial molar volume and enthalpy.

1.04 Fugacity, relation between fugacity and pressure, determination of fugacity of a real gas, variation of fugacity with temperature and pressure. Activity, dependence of activity on temperature and pressure.

1.05 Thermodynamics of mixing, Gibbs-Duhem-Margules equation, Konowaloff’s rule, Henry’s law, excess thermodynamic functions-free energy, enthalpy, entropy and volume. Determination of excess enthalpy and volume.

1.06 Chemical affinity and thermodynamic functions, effect of temperature and pressure on chemical equilibrium- vant Hoff reaction isochore and isotherm.

1.07 Third law of thermodynamics, Nernst heat theorem, determination of absolute entropies using third law, entropy changes in chemical reactions.

1.08 Three component systems-graphical representation. Solid-liquid equilibria-ternary solutions with common ions, hydrate formation, compound formation. Liquid-liquid equilibria-one pair of partially miscible liquids, two pairs of partially miscible liquids, three pairs of partially miscible liquids.

1.09 Thermodynamics of irreversible processes with simple examples. Uncompensated heat and its physical significance. Entropy production- rate of entropy production, entropy production in chemical reactions, the phenomenological relations. The principle of microscopic reversibility, the Onsager reciprocal relations. Thermal osmosis. Thermoelectric phenomena.

1.10 Bioenergetics: coupled reactions, ATP and its role in bioenergetics, high energy bond, free energy and entropy change in ATP hydrolysis, thermodynamic aspects of metabolism and respiration, glycolysis, biological redox reactions.

Unit 2: Statistical Thermodynamics **(27 Hrs)**

2.1 Permutation, probability, apriori and thermodynamic probability, Stirlings approximation, macrostates and microstates, Boltzmann distribution law, partition function and its physical significance, phase space, different ensembles, canonical partition function, distinguishable and indistinguishable molecules, partition function and thermodynamic functions, separation of partition function-translational, rotational, vibrational and electronic partition functions. Thermal de-Broglie wavelength.

2.2 Calculation of thermodynamic functions and equilibrium constants, statistical interpretation of work and heat, Sakur-Tetrode equation, statistical formulation of third law of thermodynamics, thermodynamic probability and entropy, residual entropy, heat capacity of gases - classical and quantum theories, heat capacity of hydrogen.

2.3 Need for quantum statistics, Bose-Einstein statistics: Bose-Einstein distribution, example of particles, Bose-Einstein condensation, difference between first order and higher order phase transitions, liquid helium, supercooled liquids. Fermi-Dirac distribution: examples of particles, application in electron gas, thermionic emission. Comparison of three statistics.

2.4 Heat capacity of solids- the vibrational properties of solids, Einsteins theory and its limitations, Debye theory and its limitations.

References

01. R.P. Rastogi, R.R. Misra, An Introduction to Chemical Thermodynamics, Vikas publishing house, 1996.

02. J. Rajaram, J.C. Kuriakose, Thermodynamics, S Chand and Co., 1999.

03. M.C. Gupta, Statistical Thermodynamics, New age international, 2007.

04. M.W. Zemansky, R.H. Dittman, Heat and Thermodynamics, Tata McGraw Hill, 1981.

05. P.W. Atkins, Physical Chemistry, ELBS, 1994.

06. K.J. Laidler, J.H. Meiser, B.C. Sanctuary, Physical Chemistry, 4th Edn., Houghton Mifflin, 2003.

07. L.K. Nash, Elements of Classical and Statistical Mechanics, 2nd Edn., Addison Wesley, 1972.

08. D.A. McQuarrie, J.D. Simon, Physiacl Chemistry: A Molecular Approach, University Science Books,1997

09. C. Kalidas, M.V. Sangaranarayanan, Non-equilibrium Thermodynamics, Macmillan India, 2002.

10. R.K. Murray, D.K. Granner, P. A. Mayes, V.W. Rodwell, Harper’s Biochemistry, Tata McGraw Hill,1999.

11. I. Tinoco, K. Sauer, J.C. Wang, J.D. Puglisi, Physical Chemistry: Principles and Applications in Biological Science, Prentice Hall,2002

12. F.W. Sears, G.L. Salinger, Thermodynamics, Kinetic Theory and Statistical thermodynamics, Addison Wesley, 1975.

13. J. Kestin, J.R. Dorfman, A Course in Statistical Thermodynamics, Academic Press, 1971.

SEMESTER 2

PO2C05 COORDINATION CHEMISTRY

Credits: 4 **Contact Lecture Hours: 72**

Unit 1: Structural Aspects and Bonding **(18 Hrs)**

1.1 Classification of complexes based on coordination numbers and possible geometries. Sigma and pi bonding ligands such as CO, NO, CN^-, R_3P, and Ar_3P. Stability of complexes, thermodynamic aspects of complex formation-Irving William order of stability, chelate effect.

1.2 Splitting of *d* orbitals in octahedral, tetrahedral, square planar, square pyramidal and triagonal bipyramidal fields, LFSE, *Dq* values, Jahn Teller (JT) effect, theoretical failure of crystal field theory, evidence of covalency in the metal-ligand bond, nephelauxetic effect, ligand field theory, molecular orbital theory-M.O energy level diagrams for octahedral and tetrahedral complexes without and with π-bonding, experimental evidences for pi-bonding.

Unit 2: Spectral and Magnetic Properties of Metal Complexes **(18 Hrs)**

2.1 Electronic Spectra of complexes-Term symbols of d^n system, Racah parameters, splitting of terms in weak and strong octahedral and tetrahedral fields. Correlation diagrams for d^n and d^{10-n} ions in octahedral and tetrahedral fields (qualitative approach), *d-d* transition, selection rules for electronic transition-effect of spin orbit coupling and vibronic coupling.

2.2 Interpretation of electronic spectra of complexes-Orgel diagrams, demerits of Orgel diagrams, Tanabe-Sugano diagrams, calculation of *Dq*, *B* and β (Nephelauxetic ratio) values, spectra of complexes with lower symmetries, charge transfer spectra, luminescence spectra.

2.3 Magnetic properties of complexes-paramagnetic and diamagnetic complexes, molar susceptibility, Gouy method for the determination of magnetic moment of complexes, spin only magnetic moment. Temperature dependence of magnetism-Curie's law, Curie-Weiss law. Temperature Independent Paramagnetism (TIP), Spin state cross over, Antiferromagnetism-inter and intramolecular interaction. Anomalous magnetic moments.

2.4 Elucidating the structure of metal complexes (cobalt and nickel complexes) using electronic spectra, IR spectra and magnetic moments.

Unit 3: Kinetics and Mechanism of Reactions in Metal Complexes **(18 Hrs)**

3.1 Thermodynamic and kinetic stability, kinetics and mechanism of nucleophilic substitution reactions in square planar complexes, *trans* effect-theory and applications.

3.2 Kinetics and mechanism of octahedral substitution- water exchange, dissociative and associative mechanisms, base hydrolysis, racemization reactions, solvolytic reactions (acidic and basic).

3.3 Electron transfer reactions: outer sphere mechanism-Marcus theory, inner sphere mechanism-Taube mechanism.

Unit 4: Stereochemistry of Coordination Compounds (9 Hrs)

4.1 Geometrical and optical isomerism in octahedral complexes, resolution of optically active complexes, determination of absolute configuration of complexes by ORD and circular dichroism, stereoselectivity and conformation of chelate rings, asymmetric synthesis catalyzed by coordination compounds,

4.2 Linkage isomerism-electronic and steric factors affecting linkage isomerism. Symbiosis-hard and soft ligands, Prussian blue and related structures, Macrocycles-crown ethers.

Unit 5: Coordination Chemistry of Lanthanides and Actinides (9 Hrs)

5.1 General characteristics of lanthanides-Electronic configuration, Term symbols for lanthanide ions, Oxidation state, Lanthanide contraction. Factors that mitigate against the formation of lanthanide complexes. Electronic spectra and magnetic properties of lanthanide complexes. Lanthanide complexes as shift reagents.

5.2 General characteristics of actinides-difference between $4f$ and $5f$ orbitals, comparative account of coordination chemistry of lanthanides and actinides with special reference to electronic spectra and magnetic properties.

References

01. F.A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry: A Comprehensive Text, 3rd Edn., Interscience,1972.

02. J.E. Huheey, E.A. Keiter, R.A. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Pearson Education India, 2006.

03. K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.

04. F. Basolo, R.G. Pearson, Mechanisms of Inorganic Reaction, John Wiley & Sons, 2006.

05. B.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007.

06. R.S. Drago, Physical Methods in Chemistry, Saunders College, 1992.

07. B.N. Figgis, M.A. Hitchman, Ligand Field Theory and its Applications, Wiley-India, 2010.

08. J.D. Lee, Concise Inorganic Chemistry, 4th Edn., Wiley-India, 2008

09. A.B.P. Lever, Inorganic Electronic Spectroscopy, 2nd Edn., Elsevier, 1984.

10. S. Cotton, Lanthanide and Actinide Chemistry, John Wiley & Sons, 2007.

11. T. Moeller, International Review of Science: Inorganic Chemistry, Series I, Vol VII, Butterworth, 1972.

PO2C06 ORGANIC REACTION MECHANISM

Credit: 4 **Contact Lecture Hours: 72**

Unit 1: Review of Organic Reaction Mechanisms **(9 Hrs)**

1.1 Review of organic reaction mechanisms with special reference to nucleophilic and electrophilic substitution at aliphatic carbon (SN_1, SN_2, SN_i, SE_1, SE_2, addition-elimination and elimination-addition sequences), elimination (E_1 and E_2) and addition reactions (regioselectivity: Markovnikov's addition-carbocation mechanism, anti-Markovnikov's addition-radical mechanism). Elimination vs substitution.

1.2 A comprehensive study on the effect of substrate, reagent, leaving group, solvent and neighbouring group on nucleophilic substitution(SN_2 and SN_1) and elimination (E_1 and E_2) reactions.

Unit 2: Chemistry of Carbanions **(9 Hrs)**

2.1 Formation, structure and stability of carbanions. Reactions of carbanions: C-X bond (X = C, O, N) formations through the intermediary of carbanions. Chemistry of enolates and enamines. Kinetic and Thermodynamic enolates- lithium and boron enolates in aldol and Michael reactions, alkylation and acylation of enolates.

2.2 Nucleophilic additions to carbonyls groups. Named reactions under carbanion chemistry-mechanism of Claisen, Dieckmann, Knoevenagel, Stobbe, Darzen and acyloin condensations, Shapiro reaction and Julia elimination. Favorski rearrangement.

2.3 Ylids: chemistry of phosphorous and sulphur ylids - Wittig and related reactions, Peterson olefination.

Unit 3: Chemistry of Carbocations **(9 Hrs)**

3.1 Formation, structure and stability of carbocations. Classical and non-classical carbocations.

3.2 C-X bond (X = C, O, N) formations through the intermediary of carbocations. Molecular rearrangements including Wagner-Meerwein, Pinacol-pinacolone, semi-pinacol, Dienone-phenol and Benzilic acid rearrangements, Noyori annulation, Prins reaction.

3.3 C-C bond formation involving carbocations: oxymercuration, halolactonisation.

Unit 4: Carbenes, Carbenoids, Nitrenes and Arynes **(9 Hrs)**

4.1 Structure of carbenes (singlet and triplet), generation of carbenes, addition and insertion reactions.

4.2 Rearrangement reactions of carbenes such as Wolff rearrangement, generation and reactions of ylids by carbenoid decomposition.

4.3 Structure, generation and reactions of nitrene and related electron deficient nitrene intermediates.

4.4 Hoffmann, Curtius, Lossen, Schmidt and Beckmann rearrangement reactions.

4.5 Arynes: generation, structure, stability and reactions. Orientation effect-amination of haloarenes.

Unit 5: Radical Reactions (9 Hrs)

5.1 Generation of radical intermediates and its (a) addition to alkenes, alkynes (inter & intramolecular) for C-C bond formation - Baldwin's rules (b) fragmentation and rearrangements-Hydroperoxide: formation, rearrangement and reactions. Autooxidation.

5.2 Named reactions involving radical intermediates: Barton deoxygenation and decarboxylation, McMurry coupling.

Unit 6: Chemistry of Carbonyl Compounds (9 Hrs)

6.1 Reactions of carbonyl compounds: oxidation, reduction (Clemmensen and Wolf-Kishner), addition (addition of cyanide, ammonia, alcohol) reactions, Cannizzaro reaction, addition of Grignard reagent. Structure and reactions of α, β- unsaturated carbonyl compounds involving electrophilic and nucleophilic addition-Michael addition, Mannich reaction, Robinson annulation.

Unit 7: Concerted reactions (18 Hrs)

7.1 Classification: electrocyclic, sigmatropic, cycloaddition, chelotropic and ene reactions. Woodward Hoffmann rules - frontier orbital and orbital symmetry correlation approaches - PMO method.

7.2 Highlighting pericyclic reactions in organic synthesis such as Claisen, Cope, Wittig, Mislow-Evans and Sommelet-Hauser rearrangements. Diels-Alder and Ene reactions (with stereochemical aspects), dipolar cycloaddition(introductory).

7.3 Unimolecular pyrolytic elimnination reactions: cheletropic elimination, decomposition of cyclic azo compounds, β-eliminations involving cyclic transition states such as N-oxides, acetates and xanthates.

7.4 Problems based on the above topics.

References

01. R. Bruckner, Advanced Organic Chemistry: Reaction Mechanism, Academic Press, 2002.

02. F.A. Carey, R.A. Sundberg, Advanced Organic Chemistry, Part B: Reactions and Synthesis, 5^{th} Edn., Springer, 2007.

03. W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, Cambridge University Press, 2005.

04. J. March, M.B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6^{th} Edn., Wiley, 2007.

05. A. Fleming, Frontier Orbitals and Organic Chemical Reactions, Wiley, 1976.

06. S. Sankararaman, Pericyclic Reactions-A Text Book, Wiley VCH, 2005.

07. R.T. Morrison, R.N. Boyd, S.K. Bhatacharjee, Organic Chemistry, 7^{th} Edn., Pearson, 2011.

08. J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2004.

PO2C07 CHEMICAL BONDING AND COMPUTATIONAL CHEMISTRY

Credit: 4 **Contact Lecture Hours: 72**

Unit 1: Approximate Methods in Quantum Mechanics (18 Hrs)

1.1 Many-body problem and the need of approximation methods, independent particle model. Variation method, variation theorem with proof, illustration of variation theorem using the trial function x(a-x) for particle in a 1D-box and using the trial function e^{-ar} for the hydrogen atom, variation treatment for the ground state of helium atom.

1.2 Perturbation method, time-independent perturbation method (non-degenerate case only), first order correction to energy and wave function, illustration by application to particle in a 1D-box with slanted bottom, perturbation treatment of the ground state of the helium atom. Qualitative idea of Hellmann-Feynman theorem.

1.3 Hartree Self-Consistent Field method. Spin orbitals for many electron atoms-symmetric and antisymmetric wave functions. Pauli's exclusion principle. Slater determinants. Qualitative treatment of Hartree-Fock Self-Consistent Field (HFSCF) method. Roothan's concept of basis functions, Slater type orbitals (STO) and Gaussian type orbitals (GTO), sketches of STO and GTO.

Unit 2: Chemical Bonding (18 Hrs)

2.1 Schrödinger equation for molecules. Born-Oppenheimer approximation. Valence Bond (VB) theory, VB theory of H_2 molecule, singlet and triplet state functions (spin orbitals) of H_2.

2.2 Molecular Orbital (MO) theory, MO theory of H_2^+ ion, MO theory of H_2 molecule, MO treatment of homonuclear diatomic molecules Li_2, Be_2, N_2, O_2 and F_2 and hetero nuclear diatomic molecules LiH, CO, NO and HF. Bond order. Correlation diagrams, non-crossing rule. Spectroscopic term symbols for diatomic molecules. Comparison of MO and VB theories.

2.3 Hybridization, quantum mechanical treatment of sp, sp^2 and sp^3 hybridisation. Semiempirical MO treatment of planar conjugated molecules, Hückel Molecular Orbital (HMO) theory of ethene, allyl systems, butadiene and benzene. Calculation of charge distributions, bond orders and free valency.

Unit 3: Applications of Group Theory in Chemical Bonding (9 Hrs)

3.1 Applications in chemical bonding, construction of hybrid orbitals with BF_3, CH_4, PCl_5 as examples. Transformation properties of atomic orbitals. Symmetry adapted linear combinations (SALC) of C_{2v}, C_{2h}, C_3, C_{3v} and D_{3h} point groups. MO diagram for water and ammonia.

Unit 4: Computational Chemistry (18 Hrs)

(The units 4 and 5 have been designed to expose the students to the field of computational chemistry, which has emerged as a powerful tool in chemistry capable of supplementing and complementing experimental research. The quantities which can be calculated using computational methods, how to prepare the input to get these results and the different methods that are widely used to arrive at the results are introduced here. Detailed mathematical derivations are not expected. Though computer simulations form an important part of computational chemistry, they are not covered in this syllabus.)

4.1 Introduction: computational chemistry as a tool and its scope.

4.2 Potential energy surface: stationary point, transition state or saddle point, local and global minima.

4.3 Molecular mechanics methods: force fields-bond stretching, angle bending, torsional terms, non-bonded interactions, electrostatic interactions. Mathematical expressions. Parameterisation from experiments or quantum chemistry. Important features of commonly used force fields like MM3, MMFF, AMBER and CHARMM.

4.4 Ab initio methods: A review of Hartee-Fock method. Basis set approximation. Slater and Gaussian functions. Classification of basis sets - minimal, double zeta, triple zeta, split valence, polarization and diffuse basis sets, contracted basis sets, Pople style basis sets and their nomenclature, correlation consistent basis sets.

4.5 Hartree-Fock limit. Electron correlation. Qualitative ideas on post Hartree-Fock methods-variational method, basic principles of Configuration Inetraction(CI). Perturbational methods-basic principles of Møller Plesset Perturbation Theory.

4.6 General introduction to semiempirical methods: basic principles and terminology.

4.7 Introduction to Density Functional Theory (DFT) methods: Hohenberg-Kohn theorems. Kohn-Sham orbitals. Exchange correlation functional. Local density approximation. Generalized gradient approximation. Hybrid functionals (only the basic principles and terms need to be introduced).

4.8 Model Chemistry-notation, effect on calculation time (cost).

4.9 Comparison of molecular mechanics, ab initio, semiempirical and DFT methods.

Unit 5: Computational Chemistry Calculations (9 Hrs)

5.1 Molecular geometry input-cartesian coordinates and internal coordinates, Z-matrix. Z-matrix of: single atom, diatomic molecule, non-linear triatomic molecule, linear triatomic molecule, polyatomic molecules like ammonia, methane, ethane and butane. General format of GAMESS / Firefly input file.

GAMESS / Firefly key word for: basis set selection, method selection, charge, multiplicity, single point energy calculation, geometry optimization, constrained optimization and frequency calculation.

5.2 Identifying a successful GAMESS/ Firefly calculation-locating local minima and saddle points, characterizing transition states, calculation of ionization energies, Koopmans' theorem, electron affinities and atomic charges.

5.3 Identifying HOMO and LUMO-visualization of molecular orbitals and normal modes of vibrations using suitable graphics packages.

References

01. I.N. Levine, Quantum Chemistry, 6th Edn., Pearson Education, 2009.

02. D.A. McQuarrie, Quantum Chemistry, University Science Books, 2008.

03. R.K. Prasad, Quantum Chemistry, 3rd Edn., New Age International, 2006.

04. F.A. Cotton, Chemical Applications of Group Theory, 3rd Edn., Wiley Eastern, 1990.

05. V. Ramakrishnan, M.S. Gopinathan, Group Theory in Chemistry, Vishal Publications, 1992.

06. A. S. Kunju, G. Krishnan, Group Theory and its Applications in Chemistry, PHI Learning, 2010

07. E.G. Lewars, Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, 2nd Edn., Springer, 2011.

08. J.H. Jensen, Molecular Modeling Basics, CRC Press, 2010.

09. F. Jensen, Introduction to Computational Chemistry, 2nd Edn., John Wiley & Sons, 2007.

10. A. Leach, Molecular Modelling: Principles and Applications, 2nd Edn., Longman, 2001.

11. J.P. Fackler Jr., L.R. Falvello (Eds.), Techniques in Inorganic Chemistry: Chapter 4, CRC Press, 2011.

12. K.I. Ramachandran, G. Deepa, K. Namboori, Computational Chemistry and Molecular Modeling: Principles and Applications, Springer, 2008.

13. A. Hinchliffe, Molecular Modelling for Beginners, 2nd Edn., John Wiley & Sons, 2008.

14. C.J. Cramer, Essentials of Computational Chemistry: Theories and Models, 2nd Edn., John Wiley & Sons, 2004.

15. D.C. Young, Computational Chemistry: Practical Guide for Applying Techniques to Real-World Problems, John Wiley & Sons, 2001.

Softwares

Molecular Mechanics:

1. **Arguslab** available from www.arguslab.com/
2. **Tinker** available from www.dasher.wustl.edu/ffe/

Ab initio, semiempirical and dft:

1. **Firefly / PC GAMESS** available from http://classic.chem.msu.su/gran/gamess/
2. **WINGAMESS** available from http://www.msg.ameslab.gov/gamess/

Graphical User Interface (GUI):

1. **Gabedit** available from http://gabedit.sourceforge.net/
2. **wxMacMolPlt** available from http://www.scl.ameslab.gov/MacMolPlt/
3. **Avogadro** from http://avogadro.openmolecules.net/wiki/Get_Avogadro

PO2C08 MOLECULAR SPECTROSCOPY

Credit: 3 **Contact Lecture Hours: 54**

Unit 1: Foundations of Spectroscopic Techniques (27 Hrs)

1.1 Origin of spectra: origin of different spectra and the regions of the electromagnetic spectrum, intensity of absorption, influencing factors, signal to noise ratio, natural line width, contributing factors, Doppler broadening, Lamb dip spectrum, Born Oppenheimer approximation, energy dissipation from excited states (radiative and non radiative processes), relaxation time.

1.2 Microwave spectroscopy: principal moments of inertia and classification (linear, symmetric tops, spherical tops and asymmetric tops), selection rules, intensity of rotational lines, relative population of energy levels, derivation of J_{max} , effect of isotopic substitution, calculation of intermolecular distance, spectrum of non rigid rotors, rotational spectra of polyatomic molecules, linear and symmetric top molecules, Stark effect and its application, nuclear spin and electron spin interaction, chemical analysis by microwave spectroscopy.

1.3 Infrared spectroscopy: Morse potential energy diagram, fundamentals, overtones and hot bands, determination of force constants, diatomic vibrating rotator, break down of the Born-Oppenheimer approximation, effect of nuclear spin, vibrational spectra of polyatomic molecules, normal modes of vibrations, combination and difference bands, Fermi resonance, finger print region and group vibrations, effect of H-bonding on group frequency, disadvantages of dispersive IR, introduction to FT spectroscopy, FTIR.

1.4 Raman spectroscopy: scattering of light, polarizability and classical theory of Raman spectrum, rotational and vibrational Raman spectrum, complementarities of Raman and IR spectra, mutual exclusion principle, polarized and depolarized Raman lines, resonance Raman scattering and resonance fluorescence.

1.5 Electronic spectroscopy: term symbols of diatomic molecules, electronic spectra of diatomic molecules, selection rules, vibrational coarse structure and rotational fine structure of electronic spectrum, Franck-Condon principle, predissociation, calculation of heat of dissociation, Birge and Sponer method, electronic spectra of polyatomic molecules, spectra of transitions localized in a bond or group, free electron model, different types of lasers-solid state lasers, continuous wave lasers, gas lasers and chemical laser, frequency doubling, applications of lasers, introduction to UV and X-ray photoelectron spectroscopy.

Unit 2: Resonance Spectroscopy (27 Hrs)

2.1 NMR spectroscopy : interaction between nuclear spin and applied magnetic field, nuclear energy levels, population of energy levels, Larmor precession, relaxation methods, chemical shift, representation, examples of AB, AX and AMX types, exchange phenomenon, factors influencing coupling, Karplus relationship.

2.2 FTNMR, second order effects on spectra, spin systems (AB, AB_2), simplification of second order spectra, chemical shift reagents, high field NMR, double irradiation, selective decoupling, double resonance, NOE effect, two dimensional NMR, COSY and HETCOR, ^{13}C NMR, natural abundance, sensitivity, ^{13}C chemical shift and structure correlation, introduction to solid state NMR, magic angle spinning.

2.3 EPR spectroscopy: electron spin in molecules, interaction with magnetic field, g factor, factors affecting g values, determination of g values ($g_{\parallel}$ and $g_{\perp}$), fine structure and hyperfine structure, Kramers' degeneracy, McConnell equation.

2.4 An elementary study of NQR spectroscopy.

2.5 Mossbauer spectroscopy: principle, Doppler effect, recording of spectrum, chemical shift, factors determining chemical shift, application to metal complexes, MB spectra of Fe(II) and Fe(III) cyanides.

References

01. C.N. Banwell, E.M. McCash, Fundamentals of molecular spectroscopy, 4th Edn., Tata McGraw Hill, 1994.

02. G. Aruldhas, Molecular structure and Spectroscopy, Prentice Hall of India, 2001.

03. P.W. Atkins, Physical Chemistry, ELBS,1994

04. R.S. Drago, Physical Methods in Inorganic Chemistry, Van Nonstrand Reinhold, 1965.

05. R.S. Drago, Physical Methods in Chemistry, Saunders College, 1992.

06. K.J. Laidler, J.H. Meiser, Physical Chemistry, 2nd Edn., CBS, 1999.

07. W. Kemp, NMR in chemistry-A multinuclear introduction, McMillan, 1986.

08. H. Kaur, Spectroscopy, 6th Edn., Pragati Prakashan, 2011.

09. H. Gunther, NMR spectroscopy, Wiley, 1995.

10. D.A. McQuarrie, J.D. Simon, Physical Chemistry: a molecular approach, University Science Books,1997.

11. D.N. Sathyanarayan, Electronic Absorption Spectroscopy and Related Techniques, Universities Press, 2001.

12. D.N. Sathyanarayana, Vibrational spectroscopy: Theory and Applications, New Age International, 2007

13. D.N. Sathyanarayana, Introduction To Magnetic Resonance Spectroscopy ESR,NMR,NQR, IK International, 2009.

SEMESTERS 1 AND 2

PO2P01 INORGANIC CHEMISTRY PRACTICAL

Credit: 3 **Contact Lab Hours: 54+54=108**

PART I

Separation and identification of two less familiar metal ions such as Tl, W, Se, Mo, Ce, Th, Ti, Zr, V, U and Li. Anions which need elimination not to be given. Minimum eight mixtures to be given.

PART II

Colorimetric estimation of Fe, Cu, Ni, Mn, Cr, NH_4^+, nitrate and phosphate ions.

PART III

Preparation and characterization complexes using IR, NMR and electronic spectra.

(a) Tris (thiourea)copper(I) complex

(b) Potassium tris (oxalate) aluminate (III).

(c) Hexammine cobalt (III) chloride.

(d) Tetrammine copper (II) sulphate.

(e) Schiff base complexes of various divalent metal ions.

References

01. A.I. Vogel, G. Svehla, Vogel's Qualitative Inorganic Analysis, 7th Edn., Longman,1996.

02. A.I. Vogel, A Text Book of Quantitative Inorganic Analysis, Longman, 1966.

03. I.M. Koltoff, E.B. Sandell, Text Book of Quantitative Inorganic Analysis, 3rd Edn., McMillian, 1968.

04. V.V. Ramanujam, Inorganic Semimicro Qualitative Analysis, The National Pub.Co., 1974.

PO2P02 ORGANIC CHEMISTRY PRACTICAL

Credit: 3 **Contact Lab Hours: 54+54=108**

PART I

General methods of separation and purification of organic compounds such as:

1. Solvent extraction
2. Soxhlet extraction
3. Fractional crystallization
4. TLC and Paper Chromatography
5. Column Chromatography
6. Membrane Dialysis

PART II

1. Separation of Organic binary mixtures by chemical/solvent separation methods
2. Separation of organic mixtures by TLC
3. Separation/ purification of organic mixtures by column chromatography

PART III

Drawing the structures of organic molecules and reaction schemes by ChemDraw, Symyx Draw and Chemsketch. Draw the structures and generate the IR and NMR spectra of the substrates and products in the following reactions:

1. Cycloaddition of diene and dienophile (Diels-Alder reaction)
2. Oxidation of primary alcohol to aldehyde and then to acid
3. Benzoin condensation
4. Esterification of simple carboxylic acids
5. Aldol condensation

References

01. A.I. Vogel, A Textbook of Practical Organic Chemistry, Longman, 1974.

02. A.I. Vogel, Elementary Practical Organic Chemistry, Longman, 1958.

03. F.G. Mann, B.C Saunders, Practical Organic Chemistry, 4th Edn., Pearson Education India, 2009.

04. R. Adams, J.R. Johnson, J.F. Wilcox, Laboratory Experiments in Organic Chemistry, Macmillan, 1979.

PO2P03 PHYSICAL CHEMISTRY PRACTICAL

Credit: 3 **Contact Lab Hours: 72+72 =144**

(One question each from both parts A and B will be asked for the examination)

Part A

I. Adsorption

1. Verification of Freundlich and Langmuir adsorption isotherm: charcoal-acetic acid or charcoal-oxalic acid system.
2. Determination of the concentration of the given acid using the isotherms.

II. Phase diagrams

1. Construction of phase diagrams of simple eutectics.
2. Construction of phase diagram of compounds with congruent melting point: diphenyl amine-benzophenone system.
3. Effect of (KCl/succinic acid) on miscibility temperature.
4. Construction of phase diagrams of three component systems with one pair of partially miscible liquids.

III. Distribution law

1. Distribution coefficient of iodine between an organic solvent and water.
2. Distribution coefficient of benzoic acid between benzene and water.
3. Determination of the equilibrium constant of the reaction $KI + I_2 \leftrightarrow KI_3$

IV. Surface tension

1. Determination of the surface tension of a liquid by
    a) Capillary rise method
    b) Drop number method
    c) Drop weight method
2. Determination of parachor values.
3. Determination of the composition of two liquids by surface tension measurements

Part B

Computational chemistry experiments

V. Experiments illustrating the capabilities of modern open source/free computational chemistry packages in computing single point energy, geometry optimization, vibrational frequencies, population analysis, conformational studies, IR and Raman spectra, transition state search, molecular orbitals, dipole moments etc.

Geometry input using Z-matrix for simple systems, obtaining Cartesian coordinates from structure drawing programs like Chemsketch.

References

01. J.B. Yadav, Advanced Practical Physical Chemistry, Goel publishing house, 2001.

02. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th Edn., McGraw Hill, 2009.

03. J.H. Jensen, Molecular Modeling Basics, CRC Press, 2010.

04. GAMESS documentation available from: http://www.msg.ameslab.gov/gamess/documentation.html

SEMESTER 3

PO3C09 STRUCTURAL INORGANIC CHEMISTRY

Credits: 4 **Contact Lecture Hours: 72**

Unit 1: Solid State Chemistry (18 Hrs)

1.1 Structure of solids: Imperfections in solids-point defects, line defects and plane defects. Structure of compounds of AX (Zinc blende, Wurtzite), AX_2 (Rutile, fluorite, antifluorite), A_mX_2 (Nickel Arsenide), ABX_3 (Perosvskite, Ilmenite). Spinels. Inverse spinel structures.

1.2 Solid state reactions-diffusion coefficient, mechanisms, vacancy diffusion, thermal decomposition of solid-Type I reactions, Type II reactions.

1.3 Phase transition in solids: classification of phase transitions-first and second order phase transitions, Martensitic transformations, order-disorder transitions and spinodal decomposition. Kinetics of phase transitions, sintering. Growing single crystals-crystal growth from solution, growth from melt and vapor deposition technique.

Unit 2: Electrical, Magnetic and Optical Properties (18 Hrs)

2.1 Kronig-Penney model, Free electron theory, Zone theory and MO theory of solids. Energy bands-conductors and non-conductors, intrinsic and extrinsic semiconductors. Electrons and holes. Mobility of charge carriers. Hall Effect. Pyroelectricity, piezo electricity and ferro electricity. Conductivity of pure metals.

2.2 Magnetic properties of transition metal oxides, garnets, spinels, ilmenites and perovskites, magnetoplumbites.

2.3 Optical properties-photoconductivity, photovoltaic effects, luminescence. Applications of optical properties

2.4 Super conductivity-Type I and Type II superconductors, Frolich diagram, Cooper pairs, theory of low temperature super conductors, junctions using superconductors, BCS theory of superconductivity (derivation not required). Super conducting cuprates – YbaCu oxide system, Meisner effect, conventional superconductors, organic superconductors, fullerenes, carbon nanotubes, high temperature superconductors.

Unit 3: Inorganic Chains and Rings (18 Hrs)

3.1 Chains - catenation, heterocatenation. Silicate minerals. Structure of silicates-common silicates, silicates containing discrete anions, silicates containing infinite chains, silicates containing sheets, framework silicates. Silicones. Zeolites-synthesis, structure and applications. Isopoly acids of vanadium, molybdenum and tungsten. Heteropoly acids of Mo and W. Condensed phosphates-preparation, structure and applications. Phosphate esters in biological systems. Polythiazil-one dimensional conductors.

3.2 Rings-topological approach to boron hydrides, Styx numbers. Structure and bonding in borazines, ring silicates and silicones, phosphorous-nitrogen compounds, phosphazenes. Heterocyclic inorganic ring systems-structure and bonding in phosphorous-sulphur and sulphur-nitrogen compounds. Homocyclic inorganic ring systems-structure and bonding in sulphur, selenium and phosphorous compounds.

Unit 4: Inorganic Cages and Metal Clusters (9 Hrs)

4.1 Cages: synthesis, structure and bonding of cage like structures of phosphorous. Boron cage compounds-Wade Mingos Lauher rules, MNO rule, boranes, carboranes, metallacarboranes.

4.2 Metal clusters**:** dinuclear compounds of Re, Cu and Cr, metal-metal multiple bonding in $(Re_2X_8)^{2-}$, trinuclear clusters, tetranuclear clusters, hexanuclear clusters. Polyatomic zintl anion and cations. Infinite metal chains.

Unit 5: Chemistry of Materials (9 Hrs)

5.1 Glasses, ceramics, composites, nanomaterials-preparative procedures. Sol-gel synthesis, glassy state-glass formers and glass modifiers, ceramic structures-mechanical properties, clay products, refractories- characterizations, properties and applications.

References

01. L.V. Azaroff, Introduction to Solids, Mc Graw Hill, 1984.
02. A.R. West, Solid State Chemistry and its Applications, Wiley-India, 2007.
03. D.K. Chakrabarty, Solid State Chemistry, New Age Pub., 2010.
04. D.M. Adams, Inorganic Solids: An Introduction to Concepts in Solid State Structural Chemistry, Wiley, 1974.
05. C.N.R. Rao, K.J. Rao, Phase Transitions in Solids, McGraw Hill, 2010.
06. B.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., John Wiley & sons, 2006.
07. A. Earnshaw, Introduction to Magnetochemistry, Academic Press, 1968.
08. J.E. Huheey, E.A. Keiter, R.L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Harper Collins College Pub.,1993.

09. F.A. Cotton, G. Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th Edn., Wiley-Interscience,1999.

10. K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.

11. P.C. Jain, M. Jain, Engineering Chemistry, 12th Edn., Dhanpat Rai Pub., 2006.

12. C.V. Agarwal, Chemistry of Engineering Materials, 9th Edn., B.S. Pub., 2006.

PO3C10 PHYSICAL CHEMISTRY

Credit : 4 **Contact Lecture Hours: 72**

Unit 1: Chemical Kinetics (18 Hrs)

1.1 Theories of reaction rates: Collision theory-steric factor, potential energy surfaces. Conventional transition state theory-Eyring equation. Comparison of the two theories. Thermodynamic formulation of the two theories. Thermodynamic formulation of the reaction rates. Significance of $\Delta G^{\neq}$, $\Delta H^{\neq}$ and $\Delta S^{\neq}$. Volume of activation. Effect of pressure and volume on velocity of gas reactions.

1.2 Lindemamann-Hinshelwood mechanism and RRKM theory of unimolecular reactions. Reactions in solution: factors determining reaction rates in solutions, effect of dielectric constant and ionic strength, cage effect, Bronsted-Bjerrum equation, primary and secondary kinetic salt effect, influence of solvent on reaction rates, significance of volume of activation, Hammet and Taft equation, kinetic isotope effect.

1.3 Fast reactions: relaxation, flow and shock methods, flash photolysis, NMR and ESR methods of studying fast reactions.

1.4 Acid-base catalysis: specific and general catalysis, Skrabal diagram, Bronsted catalysis law, prototropic and protolytic mechanism with examples, acidity function.

1.5 Enzyme catalysis and its mechanism, Michelis-Menten equation, effect of pH and temperature on enzyme catalysis.

1.6 Kinetics of enzyme inhibition, protein folding and pathological misfolding, muscle contraction and molecular motors.

Unit 2: Surface Chemistry and Colloids (18 Hrs)

2.1 Different types of surfaces, thermodynamics of surfaces, Gibbs adsorption equation and its verification, surfactants and micelles, general properties of emulsions, foam structure, aerosols, surface films, surface pressure and surface potential and their measurements and interpretation. Application of low energy electron diffraction and photoelectron spectroscopy, ESCA and Auger electron spectroscopy, scanning probe microscopy, ion scattering, SEM and TEM in the study of surfaces.

2.2 Adsorption: The Langmuir theory, kinetic and statistical derivation, multilayer adsorption-BET theory, Use of Langmuir and BET isotherms for surface area determination. Application of Langmuir adsorption isotherm in surface catalysed reactions, the Eley-Rideal mechanism and the Langmuir-Hinshelwood mechanism, flash desorption.

2.3 Colloids: Zeta potential, electrokinetic phenomena, sedimentation potential and streaming potential, Donnan membrane equilibrium.

Unit 3: Photochemistry **(18 Hrs)**

3.1 Quantum yield, chemical actinometry, excimers and exciplexes, photosensitization, chemiluminescence, bioluminescence, thermoluminescence, pulse radiolysis, hydrated electrons, photostationary state, dimerization of anthracene, ozone layer in the atmosphere, chemistry of photosynthesis, photography and vision.

3.2 Principle of utilization of solar energy, solar cells and their working.

3.3 Quenching of fluorescence and its kinetics, Stern-Volmer equation, concentration quenching, fluorescence and structure, delayed fluorescence, E-type and P-type, effect of temperature on emissions, photochemistry of environment, green house effect, two photon absorption spectroscopy, application of pulsed laser in measuring the dynamics of photochemical processes. Photochemistry of vision. Phototaxis and phototropism. Photochemistry of nucleic acids. Vitamin D

.

Unit 4: Nanotechnology and Green Chemistry **(18 Hrs)**

5.1 Basic principles of nanochemistry, methods of synthesis of nanomaterials, a brief study of carbon nanotubes, fullerenes, quantum dots and metal nanoparticles. Applications of nanomaterials in medicine: immunogold labelling, applications in medical diagnosis, nanobased drug delivery, biomimetic nanotechnology, DNA nanotechnology and structural biomimicry.

5.2 Principles of green chemistry, basic concepts, atom economy, twelve laws of green chemistry, principles of green organic synthesis.

5.3 Green alternatives of organic synthesis: coenzyme catalysed reactions, green alternatives of molecular rearrangements, electrophilic aromatic substitution reactions, oxidation-reduction reactions, clay catalysed synthesis, condensation reactions. Green photochemical reactions. Microwave assisted organic synthesis.

5.4 Green chemistry in the pharmaceutical industry: Ibuprofen manufacture, biocatalysis.

References

01. J. Rajaram, J.C. Kuriakose, Kinetics and Mechanisms of Chemical Transformations, Macmillan India, 2000.

02. K.J. Laidler, Chemical kinetics, 3rd Edn., Harper&Row, 1987.

03. M.R. Wright, An Introduction to Chemical Kinetics, John-Intersciece, 2007.

04. D.T. Haynie, Biological Thermodynamics, 2nd Edn., Cambridge University Press, 2008.

05. P.W. Atkins, Physical Chemistry, ELBS, 1994.

06. D.A. McQuarrie, J.D. Simon, Physical chemistry: A Molecular Approach, University Science Books, 1997.

07. A.W. Adamson, A.P. Gast, Physical Chemistry of Surfaces, 6th Edn., John Wiley & Sons, 1997.

08. K.K. Rohatgi-Mukherjee, Fundamentals of Photochemistry, 2nd Edn., New Age International,1986.

09. D.O. Cowan, R.L. Drisko, Elements of Organic Photochemistry, Plenum press, 1976.

10. P. Suppan, Chemistry and Light, Royal Society of Chemistry, 1994.

11. Z. Guo, L. Tan, Fundamentals and Applications of Nanomaterials, Artech House, 2009.

12. T. Pradeep, Nano: the Essentials, Tata McGraw Hill, 2007.

13. R.W. Kelsall, I.W. Hamely, M. Geoghegan, Nanoscale Science and Technology, John Wiley and Sons, 2005.

14. V. Kumar, An Introduction to Green Chemistry, Vishal Pub., 2007.

15. P.J. Dunn, A.S. Wells, M.T. Williams, Green Chemistry in the Pharmaceutical Industry, Wiley VCH, 2010.

16. R.A. Sheldon, I. Arends, U. Hanefeld, Green Chemistry and Catalysis, Wiley-VCH, 2007.

17. R. Ballini, Eco-Friendly Synthesis of Fine Chemicals, RSC, 2009.

PO3C11 CONCEPTS OF POLYMER CHEMISTRY

Credit: 4 **Contact Lecture Hours: 72**

Unit 1: Introduction to Polymer Science (18 Hrs)

1.1 Polymer science-history, concepts and terminology. Classification of polymers (with suitable examples) based on origin, structure, backbone, branching, action of heat, ultimate form and use, crystalline and amorphous behavior. Ladder, semi-ladder and spiro polymers.

1.2 Molecular forces in polymers - dipole forces, induction forces, dispersion forces, H-bond. Dependence of physical properties on intermolecular forces.

1.3 Polymer molecular weight-different averages, polydispersity index, molecular weight distribution curve, integral and differential distribution curve, polymer fractionation. Methods for molecular weight determination-end group analysis, colligative property measurements, membrane osmometry, vapour phase osmometry, light scattering, ultracentrifugation, viscometry and GPC.

1.4 Monomers, structure and main features of common polymers like PE, PP, PVC, PVAc, PVA, PMMA, PEMA, polylactic acid, PET, PBT, PTFE, nylon-6, nylon-6,6, Kevlar, PEEK, PES, PC, ABS, PAN, PPO, PEG, SAN, PCL, PLA, PHB, DGEBA, MF, UF, PF, PU, NR, SBR, NBR, PB, butyl rubber, polychloroprene and thiocol rubber, IIR, EPDM, CR and polyurethane elastomers.

1.5 Inorganic polymers: Types of inorganic polymers, preparation, structure and properties of polyphosphazenes, polysiloxanes, polysilanes, polygermanes and polystannanes.

Unit 2: Stereochemistry and Conformation of Polymers (18 Hrs)

2.1 Constitutional isomerism-positional isomerism and branching, substitutional isomerism (with suitable examples).

2.2 Configuration and conformation of macromolecules: stereoisomerism-optical isomerism and geometrical isomerism, configuration of polymer chains-stereoregular polymers, tacticity in polymers-monotactic and ditactic polymers. Experimental and spectroscopic methods for the determination of configuration, conformation of single macromolecule, conformation in the crystal, micro conformation in solution, ideal coil molecules in solution, compact molecules. Optically active poly(olefins), poly(amino acids), proteins. Conformational transitions.

Unit 3: Morphology and Order in Crystalline Polymers (18 Hrs)

3.1 Polymer morphology: common polymer morphologies, structural requirements for crystallinity, degree of crystallinity, crystallizability-mechanism of crystallization.

3.2 Polymer single crystals: lamellar structure of polymers-fringed micelle concept, folded chain model, adjacent re-entry model, switchboard model.

3.3 Structure of polymers: crystallized from melt-super crystalline structures, spherulitic morphology,mechanism of spherulite formation. Theories of crystallization, kinetics-Avrami equation, Hoffman's nucleation theory, the entropic barrier theory. Strain induced morphology, cold drawing, morphology changes during orientation. Theory and application of XRD, SEM and DSC in determining the crystallinity of polymers.

Unit 4: Polymer Solutions **(18 Hrs)**

4.1 Solubility of low molecular weight substances and polymers. Theories of polymer solubility, different stages of polymer solubility, non solvents, solubility of amorphous and crystalline polymers, solubility parameter concept.

4.2. Thermodynamics of polymer solution: lattice theory-advantages and limitations of lattice theory, Flory-Huggins and Flory- Krigbaum theories-advantages and limitation of FH and FK theories, corresponding state theories, Flory temperature, polymer-solvent interaction parameter, the unperturbed polymer chain, expansibility factor, entropy, enthalpy and free energy of mixing of polymer solution, phase separation in polymer systems.

4.3. The models of De Gennes and Edwards tube model (worm model), self avoiding random walk, scaling concepts in polymer systems, pearl model.

References

01. V.R. Gowariker, N.V. Viswanathan, J. Sreedhar, Polymer Science, New Age International, 2011.

02. F.W. Billmeyer Jr., Text book of Polymer Science, 3rd Edn., John Wiley & Sons, 1984.

03. L.H. Sperling, Introduction to Physical Polymer Science, 4th Edn., Wiley-Interscience, 2005.

04. J.M.G. Cowie, V. Arrighi, Polymers: Chemistry and Physics of Modern Materials, 3rd Edn., CRS Press, 2007.

05. D.I. Bower, An Introduction to Polymer Physics, Cambridge University Press, 2002.

06. M. Chanda, Introduction to Polymer Science and Chemistry, A Problem Solving Approach, CRS Press, 2006.

07. P.J. Flory, Principles of Polymer Chemistry, Cornell University Press, 1953.

08. P.G. de Gennes, Scaling Concepts in Polymer Physics, Cornell University Press, 1979.

09. I. Teraoka, Polymer Solutions: An Introduction to Physical Properties, John Wiley & Sons, 2002.
10. J.E. Mark, H.R. Allcock, R. West, Inorganic Polymers, 2nd Edn., Oxford University Press, 2005.
11. V. Chandrasekhar, Inorganic and Organometallic Polymers, Springer, 2005.

PO3C12 SPECTROSCOPIC METHODS IN CHEMISTRY

Credit : 3 **Contact Lecture Hours: 54**

Unit 1: Ultraviolet-Visible and Chirooptical Spectroscopy (9 Hrs)

1.1 Energy levels and selection rules, Woodward-Fieser and Fieser-Kuhn rules.

1.2 Influence of substituent, ring size and strain on spectral characteristics. Solvent effect, Stereochemical effect, non-conjugated interactions. Chirooptical properties-ORD, CD, octant rule, axial haloketone rule, Cotton effect.

1.3 Problems based on the above topics.

Unit 2: Infrared Spectroscopy (9 Hrs)

2.1 Fundamental vibrations, characteristic regions of the spectrum (fingerprint and functional group regions), influence of substituent, ring size, hydrogen bonding, vibrational coupling and field effect on frequency, determination of stereochemistry by IR technique.

2.2 IR spectra of C=C bonds (olefins and arenes) and C=O bonds.

2.3 Problems on spectral interpretation with examples.

Unit 3: Nuclear Magnetic Resonance Spectroscopy (18 Hrs)

3.1 Magnetic nuclei with special reference to ^{1}H and ^{13}C nuclei. Chemical shift and shielding/deshielding, factors affecting chemical shift, relaxation processes, chemical and magnetic non-equivalence, local diamagnetic shielding and magnetic anisotropy. ^{1}H and ^{13}C NMR scales.

3.2 Spin-spin splitting: AX, AX_2, AX_3, A_2X_3, AB, ABC, AMX type coupling, first order and non-first order spectra, Pascal's triangle, coupling constant, mechanism of coupling, Karplus curve, quadrupole broadening and decoupling, diastereomeric protons, virtual coupling, long range coupling-epi, peri and bay effects. NOE. NOE and cross polarization.

3.3 Simplification non-first order spectra to first order spectra: shift reagents, spin decoupling and double resonance, off resonance decoupling. Chemical shifts and homonuclear/heteronuclear couplings. Basis of heteronuclear decoupling.

3.4 2D NMR and COSY, HOMOCOSY and HETEROCOSY

3.5 Polarization transfer. Selective Population Inversion. DEPT, INEPT and RINEPT. Sensitivity enhancement and spectral editing, MRI.

3.6 Problems on spectral interpretation with examples.

Unit 4: Mass Spectrometry **(9 Hrs)**

4.1 Molecular ion: ion production methods (EI). Soft ionization methods: SIMS, FAB, CA, MALDI, PD, Field Desorption Electrospray Ionization. Fragmentation patterns-nitrogen and ring rules. McLafferty rearrangement and its applications. HRMS, MS-MS, LC-MS, GC-MS.

4.2 Problems on spectral interpretation with examples.

Unit 5: Structural Elucidation Using Spectroscopic Techniques **(9 Hrs)**

5.1 Identification of structures of unknown organic compounds based on the data from UV-Vis, IR, ^{1}H NMR and ^{13}C NMR spectroscopy (HRMS data or Molar mass or molecular formula may be given).

5.2 Interpretation of the given UV-Vis, IR and NMR spectra.

References

01. D.L. Pavia, G.M. Lampman, G.S. Kriz, Introduction to Spectroscopy, 3rd Edn., Brooks Cole, 2000.

02. A.U. Rahman, M.I. Choudhary, Solving Problems with NMR Specroscopy, Academic Press, 1996.

03. L.D. Field, S. Sternhell, J.R. Kalman, Organic Structures from Spectra, 4th Edn., John Wiley & sons, 2007.

04. C.N. Banwell, E.M. McCash, Fundamentals of Molecular Spectroscopy, 4th Edn., Tata McGraw Hill, 1994.

05. D.F. Taber, Organic Spectroscopic Structure Determination: A Problem Based Learning Approach, Oxford University Press, 2007.

06. H. Gunther, NMR Spectroscopy, 2nd Edn., Wiley, 1995.

07. R.M. Silverstein, G.C. Bassler, T.C. Morril, Spectroscopic Identification of Organic Compounds, 5th Edn., Wiley, 1991.

08. D.H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, 6th Edn., McGraw-Hill, 2008.

09. W. Kemp, Organic Spectroscopy, 2nd Edn., Macmillan, 1987.

10. F. Bernath, Spectra of Atoms and Molecules, 2nd Edn., Oxford University Press, 2005.

11. E.B. Wilson Jr., J.C. Decius, P.C. Cross, Molecular Vibrations: The Theory of Infrared and Raman Vibrational Spectra, Dover Pub., 1980.

12. Online spectral databases including RIO-DB.

SEMESTER 4

ELECTIVE COURSES

(Any 3 courses to be opted from the following courses)

PO4E01 POLYMERIZATION METHODS AND PROPERTIES OF POLYMERS

Credit : 4 **Contact Lecture Hours: 90**

Unit 1: Mechanisms of Addition Polymerization **(9 Hrs)**

1.1 Free radical addition polymerization-mechanism and kinetics of free radical addition polymerization, chain transfer, Mayo equation, thermodynamics of addition polymerization, effect of temperature, pressure, enthalpies, entropies, free energies and activation energies on polymerization, inhibition and retardation.

1.2 Ionic polymerization: common features of the two types of ionic polymerization-mechanism and kinetics of cationic polymerization, expression for the overall rate of polymerization and the number average degree of polymerization, mechanism and kinetics of anionic polymerization, expression for the overall rate of polymerization and the average degree of polymerization, living polymers.

1.3 Ziegler-Natta polymerization: Ziegler-Natta catalysts, mechanism of coordination polymerization-monometallic and bimetallic mechanisms.

Unit 2: Methods of Polymerization **(18 Hrs)**

2.1 Copolymerization: types of copolymers, the copolymer composition equation, monomer reactivity ratio and copolymer structure, influence of structural effects of monomers on monomer reactivity ratios, the Q-e scheme, synthesis of alternating, block and graft copolymers.

2.2 Step reaction(condensation) polymerization-kinetics and mechanism of step reaction polymerization, Carothers equation, number distribution and weight distribution functions, polyfunctional step reaction polymerization, prediction of gel point.

2.3 Controlled polymerization methods-nitroxide mediated polymerization, Atom Transfer Radical Polymerization(ATRP), Reversible Addition Fragmentation Termination(RAFT), electrochemical polymerization, metathetical polymerization, group transfer polymerization.

2.4 Polymerization techniques-bulk polymerization, solution polymerization, emulsion polymerization, suspension polymerization, interfacial polymerization, melt polycondensation, solution polycondensation, solid and gas phase polymerization.

Unit 3: Polymer Reactions and Polymeric Reagents **(9 Hrs)**

3.1 Polymer Reactions-hydrolysis, acidolysis, aminolysis, crosslinking, addition and substitution reactions, cyclisation reactions, reactions leading to graft and block copolymers.

3.2 A detailed study of the important polymeric reagents used for oxidation and reduction.

3.3 Polymers as supports in solid phase peptide, protein and nucleotide synthesis: a detailed survey of the various polymeric supports, their merits and limitations in the solid phase strategy of organic synthesis.

Unit 4: Polymer Testing and Characterisation **(27 Hrs)**

4.1 Thermal analysis such as dilatometry, TMA, DSC, DTA, TGA and DTG. Spectroscopic techniques such as FTIR, NMR, EPR, Raman, UV-visible, Fluorescence. X-ray diffraction.

4.2 Mechanical properties-stress, strain, elongation, yield point, yield strength, proportional limit, modulus of elasticity, ultimate strength, secant modulus, stress-strain behaviour of different types of polymers, tensile strength, stress-strain behaviour in tension compression, flexure, elongation at break, modulus, tear strength, hardness, impact properties, creep, stress-relaxation, abrasion, fatigue resistance.

4.3 Thermal properties-specific heat, heat deflection temperature, thermal conductivity, thermal expansion, brittleness temperature.

4.4 Electrical properties: dielectric strength, dielectric constant, dissipation factor, electrical resistance, volume resistivity and surface resistivity, arc resistance.

4.5 Optical properties: optical clarity, colour assessment, refractive index, luminous transmittance, haze and gloss, total internal reflection, birefringence.

Unit 5: Properties of Polymers **(18 Hrs)**

5.1 Basic determinants of polymer properties, polymer chain flexibility, factors affecting chain flexibility, glass transition temperature and crystalline melting points, transitional phenomena, first order and second order thermal transitions, molecular motion and transitions, the Boyer-Beaman rule, intermolecular bonding, external plasticization, steric factors, molecular weight variation and structure.

5.2 Molecular interpretation of the glassy state of polymers, types of mechanical deformation, structural parameters determining mechanical properties, thermal properties, optical properties, electrical properties and chemical properties.

5.3 Polymer viscoelasticity, introduction to the viscoelastic properties of polymers, some simple linear viscoelastic models-Maxwell model, Voigt model, series combination of Maxwell and Voigt model, generalized linear viscoelasticity, the

Boltzman principle, the linear viscoelastic behavior of polymer solids, creep experiments, stress relaxation experiments, stress-strain experiments, oscillatory experiments, the elastic modulus, time temperature equivalence, time-temperature superposition principle.

5.4 Rheologicalproperties of polymers-introduction to polymer melt rheology, Newtonian fluids, non-Newtonian fluids, pseudoplastic, thixotropy, St. Venant body, dilatant, complex rheological fluids, rheopectic fluids, time dependent fluids, time independent fluids, power law, Weissenberg effect, laminar flow, turbulent flow, die swell, shark skin, viscous flow, melt flow index.

5.5 Transport in polymers-diffusion, liquid and gas transport, Fick's law, theories of diffusion.

Unit 6: Research Methodology of Chemistry (9 Hrs)

6.1 The search of knowledge, purpose of research, scientific methods, role of theory, characteristics of research.

6.2 Types of research: fundamental, applied, historical and experimental research.

6.3 Chemical literature: primary, secondary and tertiary sources of literature. Classical and comprehensive reference. Literature databases: ScienceDirect, SciFinder. Chemical Abstract.

6.4 Scientific writing: research reports, thesis, journal articles, books. Types of publications: articles, communications, reviews.

6.5 Important scientific and Chemistry Journals. Impact factor.

References

01. G. Odian, Principles of Polymerization, 4th Edn., John-Interscience, 2004.
02. K.J. Saunders, Organic Polymer Chemistry, 2nd Edn., Saunders, 1888.
03. K. Matyjaszewski, T.P. Davis, Handbook of Radical Polymerization, Wiley-Interscience, 2002.
04. M. Chanda, Introduction to Polymer Science and Chemistry: A Problem Solving Approach, CRS Press, 2006.
05. M. Chanda, S.K. Roy, Plastic Technology Hand Book, Marcel Dekker, 1986.
06. J.R. Fried, Polymer Science and Technology, 2nd Edn., Prentice Hall, 2003.
07. R.P. Bown, Hand Book of Plastic Test Methods, 3rd Edn., Longman Scientific & Technical, 1988.
08. V. Shah, Hand Book of Plastic Testing Technology, Wiely-VCH, 1998.
09. J.M.G. Cowie, V. Arrighi, Polymers: Chemistry and Physics of Modern Materials, 3rd Edn., CRS Press, 2007.
10. S.V. Bhat, B.A. Nagasampagi, M. Sivakumar, Chemistry of Natural Products, Narosa, 2005.

11. T. Pradeep, Nano: the Essentials, Tata Mc Graw Hill, 2007.

12. R.L. Dominoswki, Research Methods, Prentice Hall, 1981.

13. J.W. Best, J.V. Kahn, Research in Education, 10th Edn., Pearson/Allyn&Bacon, 2006.

14. H.F. Ebel, C. Bliefert, W.E. Russey, The Art of Scientific Writing, Wiley-VCH, 2004.

PO4E02 ADVANCES IN POLYMER SCIENCE AND TECHNOLOGY

Credit: 4 **Contact Lecture Hours: 90**

Unit 1: Speciality Polymers **(18 Hrs)**

1.1 Heat resistant and fire resistant polymers: need for heat resistant polymers, improving polymers for high temperature use, need for fire resistant polymers, polymer for low fire hazards, polymers for high temperature resistance, fluoro polymers, aromatic polymers, polyether, polysulphones, polyamides, polyketones.

1.2 Polymers with electrical and electronic properties, conducting polymers-conduction mechanism, applications of conducting polymers, polyacetylene, PPP, polypyrrols and organometallic polymers, photo conducting polymers, polymers in non-linear optics, polymers with piezo, pyro, ferro electric characters, PVDF, trifluroethylene copolymers.

1.3 Ionic Polymers: classification, types of counter ion and backbone, synthesis, properties and applications. Ionic cross linking, monomers based on PE, PS, PTFE, polyelectrolytes, ionones.

1.4 Hydrophilic Polymers: Natural Polymers, Semi Synthetic Polymers, Cellulose based polymers, Synthetic Polymers, Polyacrylamide, PVA, poly(vinyl pyrrolidone).

1.5 Thermoplastic elastomers: preparation, properties and application of SBS, olefinic types, urethanes, copolymers, polyesters, 1,2-polybutadienes.

1.6 Liquid crystalline polymers: definition and synthesis, main chain liquid crystalline polymers, side chain liquid crystalline polymers, combined side chain- main chain liquid crystalline polymers, liquid crystalline polymer networks, liquid crystalline elastomers, biphasic behaviour, structure modification with liquid crystalline polymers, application of liquid crystalline polymers.

Unit 2: Polymer Compounding and Processing **(18 Hrs)**

2.1 Additives for compounding plastics, fillers, plasticizers and softners, lubricants and flow promoters, antiaging additives, flame retarders, colorants, blowing agents, UV stabilizers, requirement and functions of each ingredient.

2.2 Compounding ingredients for rubber: fillers-reinforcing, semi reinforcing and non reinforcing, peptizers, vulcanizing agents, activators, accelerators, anti-oxidants, antiozonants, pigments, tackifiers, blowing agents, bonding agents and processing aids. Vulcanization of rubber, types of vulcanisation, rheograph, cure time, scorch time.

2.2 Compound development-formulation of mixes, compounding for specific applications, ozone resistance, heat resistance, weather, oil and radiation resistance, impermeability, medical application, low temperature properties, electrical and optical applications.

2.3 Processing methods for the manufacture of products with dry rubber-blending and mastication, master batching of polymers, mixing and compounding in mills and internal mixers, calendaring, sheeting, fabric coating, extension, moulding, batch curing, cold curing, continuous vulcanization methods-high pressure steam, hot air tunnel, molten salt bath, fluidized bed, continuous drum care and microwave curing.

2.4 Finishing rubber products-flash and spew removal, punching, grinding, shot blasting painting and lacquering and chemical surface treatment.

2.5 Processing methods of plastics-methods of mixing-injection, reaction injection, compression and transfer moulding, extrusion, calendaring, thermoforming, blow moulding, rotational moulding and slush moulding.

Unit 3: Polymer Blends and Composites (18Hrs)

3.1 Polymer blends: definition and importance of blending, Blending techniques-solution mixing, mechanical mixing, latex blending, mechano chemical blending.

3.2 Compatibility of polymer in solution, determination of mutual solubility of polymers, miscibility through specific interactions, copolymer effect, phase diagrams of polymer-polymer systems. LCST and UCST behaviour, binodal and spinodal curves, critical point, phase separation mechanisms.

3.3 Thermodynamic treatment of phase behaviour of polymer mixtures, Flory-Huggins theory, blend morphology, morphology generation and control, capillary number, morphology characterization techniques, commercial blends and their applications.

3.4 Methods for determining polymer-polymer miscibility, criteria for establishing miscibility, dielectric methods, microscopy, cloud point method, rheological methods, dilatometry, viscosity methods, free volume measurement, volume of mixing, mutual solvent method, heat of mixing, melting point depression, inverse gas chromatography, specific advantages of miscible and immiscible polymer blends.

3.5 Compatibilisation-fundamental concepts, general routes to compatibility, types of compatibilisers-addition of graft of block copolymers, insitu formed copolymers, separately added copolymers, reactive compatibilisation by low molecular weight additives, compatibilisation theories-contributions of Noolandi, Hong and Leibler.

3.6 Polymer composites: definition and classification, role of fibre and matrix in improving composite properties, mechanics of short and long fibre composites, bonding between fibre and matrix-functions of bonding agents, critical fibre length in short fiber composites, failure mechanism in composites.

Unit 4: Fibre Science and Technology **(9 Hrs)**

4.1 Definition of fibres, classification and nomenclature of fibres, structural principles of fibre forming polymers, regularity, shape and interaction, repeat length, chain directionality, single chain formation, and chain stiffness.

4.2 Chemical composition, production and use of vegetable fibres such as cotton, flax, linen, coir, sisal, animal fibre such as wool and silk, mineral fibre such as asbestos and glass, microstructure of natural fibre.

4.3 Chemical composition, production and properties of man-made fibres such as viscose, rayon, cellulose acetate, nylon-6,6, nylon-6, carbon fibre, polyesters, acrylic fibres.

4.4 Fundamentals and general techniques of fibre spinning (melt, wet and dry spinning), fibre drawing, heat setting, texturing of fibres.

Unit 5: Adhesives and Surface Coating **(18 Hrs)**

5.1 Mechanism of adhesion, mechanical interlocking, inter-diffusion, adsorption and surface reaction, electrostatic attraction.

5.2 Surface and interfacial properties, surface topography, surface tension and energy, wetting and setting, thermodynamic work of adhesion.

5.3 Surface treatment, CASING (crosslinking by activated species of inert gas) or plasma treatment, corona discharge, acid etching, transcrystallization growth, surface grafting, treatment for fluorocarbon polymers and metals.

5.4 Tack and auto adhesion, pressure sensitive adhesion, tackifiers, rate of peel and temperature, effects in pressure sensitive adhesion, auto adhesion of elastomers, effect of molecular weight on tack and green strength of NR, effect of contact time and pressure on the tack of elastomers.

5.5 Physical nature of adhesives, hot melt, solutions, aqueous dispersion, activated adhesives, film adhesive, pressure sensitive adhesives, polymerising types, radiation curable.

Unit 6: Latex technology **(9 Hrs)**

6.1 Introduction to latices, classification of latices, comparisons and contrasts between polymer latices and polymer solutions, investigation of latex properties-TSC, DRC, pH, alkalinity, colloidal stability, KOH number, VFA, surface free energy, density, residues.

6.2 Preservation and concentration of natural rubber latex, types of dipping processes, Dunlop process

Unit 7: Polymer Recycling **(9 Hrs)**

6.1 Reprocessing of thermoplastic recyclates, contaminants.

6.2 Recycling techniques, size reduction, washing, identification and sorting of plastics, agglomeration, other methods of recycling and waste disposal options, chemical recycling, thermal conversion technologies.

References

01. D.R. Paul, Polymer Blends, Vol 1 and Vlol 2, Academic Press, 1978
02. O. Olabisi, L.M. Robeson, M.T. Shaw, Polymer-Polymer Miscibility, Academic Press, 1979.
03. K.K. Chawla, Composite Materials: Science and Engineering, Springer, 1998.
04. F.R. Jones, Hand Book of Polymer-Fibre Composites, Longman Scientific and Technical, 1994.
05. R.W. Dyson, Speciality Polymers, Chapmann and Hall, 1987.
06. A.H. Frazer, High Temperature Resistant Polymers, Interscience, 1968.
07. J.I. Kroschwitz, Encyclopedia of Polymer Science and Engineering Vol.10, Wiley, 1990.
08. J.A. Brydson, Plastic Materials, Butterworths-Hieneman, 1999.
09. F.W. Billmeyer Jr., Text book of Polymer Science, 3rd Edn., John Wiley & Sons, 1984.
10. W.A.H. Walker, Polymer Conversion, Applied Science, 1975.
11. R.W. Moncrieff, Man-made Fibres, Wley, 1970.
12. I. Skeist, Handbook of Adhesives, 2nd Edn., Van Nostrand Reinhold, 1977.
13. J. Shields, Adhesives Handbook, Butterworths, 1970.
14. A. Pizzi, Wood Adhesives:Chemistry and Technology, Marcel Dekker, 1989.
15. D.C. Blackley, Polymer Latices, Vol.1,2,&3. 2nd Edn., Springer, 1997.

PO4E03 ADVANCED ORGANIC CHEMISTRY

Credit : 4 **Contact Lecture Hours: 90**

Unit 1: Organic Synthesis via Oxidation and Reduction (18 Hrs)

1.1 Survey of organic reagents and reactions in organic chemistry with special reference to oxidation and reduction. Metal based and non-metal based oxidations of (a) alcohols to carbonyls (Chromium, Manganese, aluminium and DMSO based reagents) (b) alkenes to epoxides (peroxides/per acids based)-Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation (c) alkenes to diols (Manganese and Osmium based)-Prevost reaction and Woodward modification (d) alkenes to carbonyls with bond cleavage (Manganese and lead based, ozonolysis) (e) alkenes to alcohols/carbonyls without bond cleavage-hydroboration-oxidation, Wacker oxidation, selenium/chromium based allylic oxidation (f) ketones to ester/lactones- Baeyer-Villiger oxidation.

1.2 (a) Catalytic hydrogenation (Heterogeneous: Palladium/Platinum/Rhodium and Nickel. Homogeneous: Wilkinson). (b) Metal based reductions- Birch reduction, pinacol formation, acyloin formation (c) Hydride transfer reagents from Group III and Group IV in reductions - $LiAlH_4$, DIBAL-H, Red-Al, $NaBH_4$ and $NaCNBH_3$, selectrides, trialkylsilanes and trialkylstannane. Meerwein-Pondorff-Verley reduction. Baker's yeast.

Unit 2: Modern Synthetic Methods and Reagents (18 Hrs)

2.1 Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction, Ugi reaction, Noyori reaction. Brook rearrangement. Tebbe olefination. Metal mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki, Suzuki-Miyaura, Negishi-Sonogashira, Nozaki-Hiyama, Buchwald-Hartwig, Ullmann and Glaser coupling reactions. Wohl-Ziegler reaction. Reagents such as NBS, DDQ and DCC. Gilmann reagent.

2.2 Introduction to multicomponent reactions-Click reactions.

Unit 3: Construction of Carbocyclic and Heterocyclic Ring Systems (9 Hrs)

3.1 Different approaches towards the synthesis of three, four, five and six-membered rings. Photochemical approaches for the synthesis of four membered rings-oxetanes and cyclobutanes, ketene cycloaddition (inter and intra molecular), Pauson-Khand reaction, Volhardt reaction, Bergman cyclization, Nazarov cyclization, Mitsunobu reaction, cation-olefin cyclization and radical-olefin cyclization.

3.2 Inter-conversion of ring systems (contraction and expansion)-Demjenov reaction, Reformatsky reaction. Construction of macrocyclic rings-ring closing metathesis.

3.3 Formation of heterocyclic rings: 5-membered ring heterocyclic compounds with one or more than one hetero atom like N, S or O - pyrrole, furan, thiophene, imidazole, thiazole and oxazole.

Unit 4: Protecting Group Chemistry (9 Hrs)

4.1 Protection and deprotection of hydroxy, carboxyl, carbonyl, and amino groups. Chemo and regio selective protection and deprotection. Illustration of protection and deprotection in synthesis.

4.2 Protection and deprotection in peptide synthesis: common protecting groups used in peptide synthesis, protecting groups used in solution phase and solid phase peptide synthesis (SPPS).

4.3 Functional equivalence and reactivity Umpolung. Role of trimethyl silyl group in organic synthesis.

Unit 5: Reterosynthetic Analysis (9 Hrs)

5.1 Basic principles and terminology of reterosynthesis: synthesis of aromatic compounds, one group and two group C-X disconnections, one group C-C and two group C-C disconnections.

5.2 Amine and alkene synthesis: important strategies of retrosynthesis, functional group transposition, important functional group interconversions. Enantioselective synthesis of Corey lactone, longifolene and luciferin. Umpolung equivalent - Peterson olefination, enolate formation, Ireland method.

Unit 6: Biosynthesis and Biomimetic Synthesis (9 Hrs)

6.1 Basic principles of the biosynthesis of terpenes, steroids, alkaloids, carbohydrates, proteins and nucleic acids. Biosynthesis of cholesterol, α- terpineol, morphine, glucose and phenyl alanine. Biogenesis of isoprenoids and alkaloids. Biomimetic synthesis of progesterone and spatreine.

Unit 7: Dendrimers and Dentritic Polymers (18 Hrs)

5.1 Basic concepts and terminology: Dendrons, star shaped and starbust polymers-dendrimer formation and dendrimer generations-various types of dendrimers.

5.2 Synthesis of dendrimers-convergent and divergent approaches-methods and mechanism of dendrimer synthesis. Properties of dendrimers-polydispersity, mechanical properties, viscoelastic properties. Determination of physical properties.

5.3 Characterisation of dendrimers: GPC, osmosis, TG, DSC, magnetic resonance spectroscopy: proton and carbon-13 NMR methods. Mass spectral studies-MALDI-TOF.

5.4 Dendritic macromolecules: hypergrafted and hyperbranched polymers, definition and classification, synthesis: methods and mechanism, characterization, properties, applications.

References

01. M.B. Smith, Organic Synthesis, 3rd Edn., Wavefunction Inc., 2010.

02. F.A. Carey, R.I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edn., Springer, 2007.

03. S. Warren, P. Wyatt, Organic Synthesis: The Disconnection Approach, 2nd Edn., Wiley, 2008.

04. V.K. Ahluwalia, Oxidation in Organic Synthesis, CRC Press, 2012.

05. I. Ojima, Catalytic Asymmetric Synthesis, 3rd Edn., John Wiley & sons, 2010.

06. W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, 4th Edn., Cambridge University Press, 2004.

07. J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2001.

08. R. Noyori, Asymmetric Catalysis in Organic Synthesis, John Wiley & Sons, 1994.

09. L. Kuerti, B. Czako, Strategic Applications of Named Reactions in Organic Synthesis, Elsevier Academic Press, 2005.

10. R.O.C. Norman, J.M. Coxon, Principles of Organic Synthesis, 3rd Edn., Chapmann and Hall, 1993.

11. V.K. Ahluwalia, L.S. Kumar, S. Kumar, Chemistry of Natural Products, CRS Press, 2007.

12. J.M.J. Frechet, D.A. Tomalia, Dendrimers and Other Dentritic Polymers, Wiley, 2001.

13. J.M.J. Frechet, C.J. Hawker, Comprehensive Polymer Science, 2nd Edn., Pergamon, 1996.

PO4E04 ANALYTICAL CHEMISTRY

Credit: 4 **Contact Lecture Hours: 90**

Unit 1: Instrumental Methods **(36 Hrs)**

1.1 Electrical and nonelectrical data domains-transducers and sensors, detectors, examples for piezoelectric, pyroelectric, photoelectric, pneumatic and thermal transducers. Criteria for selecting instrumental methods-precision, sensitivity, selectivity, and detection limits.

1.2 Signals and noise: sources of noise, S/N ratio, methods of enhancing S/N ratio-hardware and software methods.

1.3 Electronics: transistors, FET, MOSFET, ICs, OPAMs. Application of OPAM in amplification and measurement of transducer signals.

1.4 UV-Vis spectroscopic instrumentation: types of optical instruments, components of optical instruments-sources, monochromators, detectors. Sample preparations. Instrumental noises. Applications in qualitative and quantitative analysis.

1.5 Molecular fluorescence and fluorometers: photoluminiscence and concentration-electron transition in photoluminescence, factors affecting fluorescence, instrumentation details. Fluorometric standards and reagents. Introduction to photoacoustic spectroscopy.

1.6 IR spectrometry: instrumentation designs-various types of sources, monochromators, sample cell considerations, different methods of sample preparations, detectors of IR-NDIR instruments. FTIR instruments. Mid IR absorption spectrometry. Determination of path length. Application in qualitative and quantitative analysis.

1.7 Raman Spectrometric Instrumentation: sources, sample illumination systems. Application of Raman Spectroscopy in inorganic, organic, biological and quantitative analysis.

1.8 NMR Spectrometry-magnets, shim coils, sample spinning, sample probes (^{1}H, ^{13}C, ^{32}P). Principle of MRI.

Unit 2: Sampling **(18 hrs)**

2.1 The basis and procedure of sampling, sampling statistics, sampling and the physical state, crushing and grinding, the gross sampling, size of the gross sample, sampling liquids, gas and solids (metals and alloys), preparation of a laboratory sample, moisture in samples-essential and non essential water, absorbed and occluded water, determination of water (direct and indirect methods).

2.2 Decomposition and dissolution, source of error, reagents for decomposition and dissolution like HCl, H_2SO_4, HNO_3, $HClO_4$, HF, microwave decompositions, combustion methods, use of fluxes like Na_2CO_3, Na_2O_2, KNO_3, NaOH, $K_2S_2O_7$,

B_2O_3 and lithium metaborate. Elimination of interference from samples-separation by precipitation, electrolytic precipitation, extraction and ion exchange. Distribution ratio and completeness of multiple extractions. Types of extraction procedures.

Unit 3: Applied Analysis **(9 hrs)**

3.1 Analytical procedures involved in environmental monitoring. Water quality-BOD, COD, DO, nitrite, nitrate, iron, fluoride.

3.2 Soil-moisture, salinity, colloids, cation and anion exchange capacity.

3.3 Air pollution monitoring sampling, collection of air pollutants-SO_2, NO_2, NH_3, O_3 and SPM.

3.4 Analysis of metals, alloys and minerals. Analysis of brass and steel. Analysis of limestone. Corrosion analysis.

Unit 4: **Capillary Electrophoresis and Capillary Electro-chromatography** **(9 Hrs)**

4.1 Capillary electrophoresis-migration rates and plate heights, instrumentation, sample introduction, detection(indirect)-fluorescence, absorbance, electrochemical, mass spectrometric, applications. Capillary gel electrophoresis. Capillary isotachophoresis. Isoelectric focusing.

4.2 Capillary electro chromatography-packed columns. Micellar electro kinetic chromatography.

Unit 5: Process instrumentation **(9 Hrs)**

5.1 Automatic and automated systems, flow injection systems, special requirements of process instruments, sampling problems, typical examples of C, H and N analysers.

Unit 6: Aquatic Resources **(9 Hrs)**

6.1 Aquatic resources: renewable and non renewable resources, estimation, primary productivity and factors affecting it, regional variations.

6.2 Desalination: principles and applications of desalination-distillation, solar evaporation, freezing, electrodialysis, reverse osmosis, ion exchange and hydrate formation methods. Relative advantages and limitations. Scale formation and its prevention in distillation process.

6.3 Non-renewable resources: inorganic chemicals from the sea-extraction and recovery of chemicals, salt from solar evaporation.

References

01. J.M. Mermet, M. Otto, R. Kellner, Analytical chemistry, Wiley-VCH, 2004.

02. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8^{th} Edn., Saunders College Pub., 2007.

03. R.D. Brownn, Introduction to Instrumental Analysis, McGraw-Hill, 1958.

04. H.H. Willard, L.L. Merritt, J.A. Dean, Instrumental Methods of Analysis, Van Nostrand, 1974.

05. G.D. Christian, J.E. O'Reilly, Instrumental Analysis, Allyn & Bacon, 1986.

06. J.H. Kennedy, Analytical Chemistry: principles, Saunders College Pub., 1990.

07. J.G. Dick, Analytical Chemistry, R.E. Krieger Pub., 1978.

08. E.D. Howe, Fundamentals of Water Desalination, Marcel Dekker, 1974.

09. H.G. Heitmann, Saline Water Processing, VCH, 1990.

SEMESTERS 3 AND 4

PO4P04 POLYMER PREPARATIVE PRACTICAL

Credit: 3 **Contact Lab Hours: 54+54 =108**

PART I: Preparation of Polymers

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

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

PART II: Latex Analysis

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

References

01. E.A. Collins, J. Bares, F.W. Billmeyer, Experiments in Polymer Science, Wiley-Interscience, 1973.

02. S.H. Pinner, A Practical Course in Polymer Chemistry, Pergamon, 1961.

03. D. Braun, H. Cherdron, W. Kern, Practical Macromolecular Organic Chemistry, 3rd Edn, Harwood Academic Pub., 1984.

04. S.R. Sandler, W. Karo, Polymer Synthesis, Vol.1, Academic Press, 1992.

05. S.R. Sandler, W. Karo, Polymer Synthesis, Vol.2, Academic Press, 1993.

06. S.R. Sandler, W. Karo, Polymer Synthesis, Vol.3, Academic Press, 1998.

07. D. C. Blackley, Polymer Latices, Vol.1, 2 & 3, 2nd Edn., Springer, 1997.

08. W.C. Wake, Analysis of Rubbers and Rubber like Polymers, 2nd Edn, Wiley-Interscience, 1969.

PO4P05 POLYMER CHARACTERIZATION PRACTICAL

Credit: 3 **Contact Lab Hours: 54+54=108**

PART I

Osmometry -determination of molecular weight of polymers by osmotic pressure method, viscometry -same with dilute solution viscometry of polymers, same with GPC.

PART II

Thermoanalytical methods-determination of phase transition in polymers by TGA and DTA, determination of T_g, T_m and crystallinity by DSC.

PART III

Potentiometric and conductometric titrations of polyelectrolyte solutions, pH measurements of polyelectrolyte solutions chemical methods.

PART IV

IR and NMR analysis of polymers.

PART V

Chromatographic techniques (paper, thin layer, gas and HPLC), for the analysis of polymers.

PART VI

End group analysis, determination of acid value, swelling studies, determination of crosslink density from swelling method, total sulphur, zinc sulphide products at each stage of the products synthesized by the above methods.

PART VII

Measurement of electrical and optical properties of polymers

PART VIII

Systematic identification of virgin and compounded polymer sample:

Rubbers-NR, SBR, NBR, butyl rubber, neoprene etc.

Plastics-PE, PP, PVC, nylon, PS, PMMA etc.

References

01. J. Mitchell, Applied Polymer Analysis and Characterization, Hanser, 1992.
02. H.H. Willard, L.L. Merrit, J.A. Dean, Instrumental Methods of Analysis, 3rd Edn., Van Nostrand, 1963.
03. G.C. Ives, J.A. Mead, M.M. Riley, Handbook of Plastics Test Methods, CRC Press, 1971.
04. R.P. Brown, Handbook of Plastics Test Methods, 3rd Edn., Longman Scientific and Technical, 1988.

PO4P06 POLYMER PROCESSING AND TESTING PRACTICAL

Credit: 3 **Contact Lab Hours: 72+72=144**

1. Compounding and moulding-Plastics compounding, rubber compounding, latex compounding.

2. Cure characterization.

3. Polymer processing (extrusion, injection moulding, compression moulding, calendaring, thermoforming)

4. Composite preparation and characterization

5. Testing of mechanical properties of rubbers, plastics and composite (tensile, compression, shear,abrasion, tear, impact, hardness, flexural etc.)

    a. Stress-strain in tension, compression, flexure and shear
    b. Tensile strength
    c. Young's modulii
    d. Tear strength
    e. Abrasion resistance
    f. Flex resistance
    g. Heat build up
    h. Impact strength
    i. Flexural tests
    j. Resilience
    k. HDT
    l. Hardness

References

01. R.P. Brown, Physical Testing of Rubber, 3rd Edn, Springer, 1996.
02. V. Shah, Handbook of Plastic Testing Technology, 2nd Edn, John Wiley & Sons, 1998.
03. R. Brown, Handbook of Polymer Testing, Rapra Technology, 2002.
04. R.P. Brown, Handbook of Plastics Test Methods, 3rd Edn, Longman Scientific and Technical, 1988.