MASTER OF SCIENCE (M.Sc.)

IN

POLYMER CHEMISTRY

PROGRAM STRUCTURE AND SYLLABUS

2019-20 ADMISSION ONWARDS

(UNDER MAHATMA GANDHI UNIVERSITY PGCSS REGULATIONS 2019)

BOARD OF STUDIES IN CHEMISTRY (PG)

MAHATMA GANDHI UNIVERSITY

2019

PREFACE

I feel privileged in presenting the revised curriculum and syllabus of **CH05 M. Sc. POLYMER CHEMISTRY PROGRAM** for favour of approval by the Faculty of Science and Academic Council of Mahatma Gandhi University, Kottayam, Kerala, India.

With effect from 2012-2013 academic year, the University has introduced the Credit & Semester system for all the PG programmes in affiliated colleges/institutions, as per Mahatma Gandhi University PG Programme Regulations for Credit& Semester System 2011(MGU-CSS-PG). The University has decided to revise the syllabus and curriculum as per University Order No.7484/Ac.AIX/syllabus revision committee dated 22/02/2018 with effect from 2019 academic year.

Based on the guidelines of M. G. University for Credit & Semester System, the PGBOS prepared draft proposals for revised curricula and syllabi of all the five branches of M.Sc. Chemistry. With the active participation of resource persons and teacher representatives from all the colleges, a three-day workshop was conducted during 17-19 January 2019 at St. Thomas College, Palai for revising the existing curricula and syllabi. Finalisation of the proposal of the restructured curricula and syllabi was made by the BOS by incorporating many of the suggestions raised by the participants in the workshop.

With dedicated efforts, wholehearted support and involvement of all the members of the BOS, the task of preparing the curricula and syllabi and bringing it out in the present form was made possible. I sincerely express my whole-hearted gratitude to all the fellow members of the BOS for their endless help, cooperation and encouragement showered on me for the completion of this great task. I am also thankful to all Resource Persons and Teacher Representatives from Postgraduate Chemistry Departments of various colleges for their active participation and fruitful suggestions during the three-day workshop.

Dr. GEETHA P

Chairperson, PG Board of Studies in Chemistry

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General Information

M. Sc. Chemistry Degree Program

(Mahatma Gandhi University Regulations PGCSS2019 from 2019-20 Academic Year)

1. Aim of the Programme

Chemistry, being central to all other sciences, its study provides a fundamental insight into the changes taking place in and around our fascinating nature. No one can understand the modern world without the basic knowledge of Chemistry and its advanced study help us to have a thorough knowledge of the entire world.

Through lectures, laboratory work, exercises, project work, and its independent master's thesis, students will gain knowledge about relevant working methods for research, industry, administration, and education. The Master's degree program in Chemistry lays the foundation for doctoral programs in Chemistry.

2. Eligibility Criteria for admissions

Graduation in Chemistry/Petrochemicals with not less than CCPA of 5.00 out of 10.00 in Core Group (Core + Complementary + Open Courses).

Relaxation in Marks in the qualifying examination:

1. For SC/ST category, a pass in the qualifying examination is the minimum requirement for admission.
2. For OEC category CCPA of 4.5 in the qualifying examination is required.

3. Medium of instruction

English

Assessment

The weightage for internal & external evaluation of theory/practical/ project/comprehensive viva-voce is 5 & 15 and the maximum Weighted Grade Point (WGP) is 25 & 75 respectively, (ratio 1:3)

Pattern of Questions

Sl.No.	Type of Questions	Weight	Number of questions to be answered
1.	Short Answer type questions	1	8 out of 10
2	Short essay/ problem solving type questions	2	6 out of 8
3.	Long Essay type questions	5	2 out of 4

Direct Grading System

Direct Grading System based on a 7–point scale is used to evaluate the performance (External and Internal Examination of students)

For all courses (theory & practical)/semester/overall programme Letter grades and GPA/SGPA/CGPA are given on the following scale:

Range	**Grade**	**Indicator**
4.50 to 5.00	A+	Outstanding
4.00 to 4.49	A	Excellent
3.50 to 3.99	B+	Very good
3.00 to 3.49	B	Good (Average)
2.50 to 2.99	C+	Fair
2.00 to 2.49	C	Marginal
up to 1.99	D	Deficient(Fail)

Minimum **C grade** is required for pass in a course.

Evaluation first stage - Both internal and external (to be done by the teacher)

Grade	**Grade Points**
A+	5
A	4
B	3
C	2
D	1
E	0

Weightage Distribution for External and Internal Examination

Theory-External

Maximum weight & Maximum Weighted Grade Point (WGP) for external evaluation is **30** and**150** respectively.

Theory-Internal (Components and Weightage)

	Components	**Weightage**
1	Assignment	1
ii	Seminar	2
iii	Best Two Test papers	1 each (2)
	Total	**5**

Practical-External (Components and Weightage)

Components	**Weightage**
Written / Lab test	10
Record	2
Viva	3
Total	**15**

Practical-Internal (Components and Weightage)

Components	**Weightage**
Written/Lab test	3
Lab involvement	1
Viva	1
Total	**5**

Project- External (Components and Weightage)

Components	**Weightage**
Relevance of the topic and analysis	2
Project content and presentation	8
Project viva	5
Total	**15**

Project- Internal (Components and Weightage)

Components	Weightage
Relevance of the topic and analysis	1
Project content and presentation	3
Project viva	1
Total	**5**

Comprehensive viva-voce (External)-components and weightage

Components	Weightage
Course viva (all courses from first semester to fourth semester)	15
Total	**15**

Comprehensive viva (Internal) - Components and Weightage

Components	Weightage
Course viva (all courses from first semester to fourth semester)	5
Total	**5**

4. **Faculty under which the Degree is awarded**

   Science

5. **Note on compliance with the UGC minimum standards for the conduct and award of Post Graduate Degrees**

Credit and Semester system is followed in this program. The program has 4 semesters with 18 weeks in each semester. In each week, there are 15 lecture hours and 10 laboratory hours. In each semester there are 270 lecture hours and180 practical hours; thus a total of 450 calendar hours in each semester which is in compliance with the minimum 390 hours stipulated by the UGC.

PROGRAMME STRUCTURE

	Code	Course	Hours / Week	Total Hours	Credit
Semester 1	CH 50 01 01	Organometallics and Nuclear Chemistry	4	72	4
	CH 50 01 02	Structural and Molecular Organic Chemistry	4	72	4
	CH 50 01 03	Quantum Chemistry and Group Theory	4	72	4
	CH 50 01 04	Thermodynamics, Kinetic Theory and Statistical Thermodynamics	3	54	4
	CH 50 02 05	Inorganic Chemistry Practical-1	3	54	Evaluation at the end of second semester
	CH 50 02 06	Organic Chemistry Practical-1	3	54	
	CH 50 02 07	Physical Chemistry Practical-1	4	72	
		Total	**25**	**450**	**16**
Semester 2	CH 50 02 01	Coordination Chemistry	4	72	4
	CH 50 02 02	Organic Reaction Mechanisms	4	72	4
	CH 50 02 03	Chemical Bonding and Computational Chemistry	4	72	3
	CH 50 02 04	Molecular Spectroscopy	3	54	3
	CH 50 02 05	Inorganic Chemistry Practical-1	3	54	3
	CH 50 02 06	Organic Chemistry Practical-1	3	54	3
	CH 50 02 07	Physical Chemistry Practical-1	4	72	3
		Total	**25**	**450**	**23**
Semester 3	CH 50 03 01	Structural Inorganic Chemistry	4	72	4
	CH 05 03 02	Chemical Kinetics and Surface Chemistry	4	72	4
	CH 05 03 03	Concepts of Polymer Chemistry	4	72	4
	CH 50 03 04	Spectroscopic Methods in Chemistry	3	54	4
	CH 05 04 05	Polymer Preparative Practical-2	3	54	Evaluation at the end of fourth semester
	CH 05 04 06	Polymer Characterization Practical-2	3	54	
	CH 05 04 07	Polymer Processing and Testing Practical-2	4	72	
		Total	**25**	**450**	**16**

		Elective(Group A)			
Semester 4	CH 88 04 01	Properties and Characterisation Methods of Polymers	5	90	4
	CH 88 04 02	Advances in Polymer Science and Technology	5	90	4
	CH 88 04 03	Advanced Organic Chemistry	5	90	4
		Elective(Group B)			
	CH 89 04 01	Medicinal Chemistry	5	90	4
	CH 89 04 02	Advances in Polymer Science and Technology	5	90	4
	CH 89 04 03	Analytical Chemistry	5	90	4
	CH 05 04 04	Project			2
	CH 05 04 05	Polymer Preparative Practical-2	3	54	3
	CH 05 04 06	Polymer Characterization Practical-2	3	54	3
	CH 05 04 07	Polymer Processing and Testing Practical-2	4	72	3
	CH 05 04 08	Viva			2
		Total	**25**	**450**	**25**
GRAND TOTAL					**80**

SEMESTER 1

CH 50 01 01 ORGANOMETALLICS AND NUCLEAR CHEMISTRY

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

Objective of the course

The learners should be able to apply and analyse the methods of synthesis and the mechanism of selected catalytic organic reactions from the structure-bonding aspects and reactivity of simple organometallic compounds, the functions of transition metal ions in biological systems and the applications of radioactive isotopes in various fields.

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

1.1 Hapto nomenclature of organometallic compounds, organometallic compounds with linear pi donor ligands-olefins, acetylenes, dienes and allyl complexes-synthesis, structure and bonding.

1.2 Synthesis and structure of complexes with cyclic pi donors, metallocenes and cyclic arene complexes, bonding in ferrocene and dibenzenechromium, carbene and carbyne complexes.

1.3 Metal carbonyls: CO as a π-bonding ligand, synergism, 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. IR spectral studies of bridging and non-bridging CO ligands.

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- concerted addition, S_N2, radical and ionic mechanisms. Reductive elimination- binuclear reductive elimination and σ-bond metathesis. Oxidative coupling and reductive decoupling. Insertion (migration) and elimination reactions – insertions of CO and alkenes, insertion into M−H versus M−R, α, β, γ and δ eliminations.

2.3 Redistribution reactions, fluxional isomerism of allyl, cyclopentadienyl and allene systems.

Unit 3: Catalysis by Organometallic Compounds (18 Hrs)

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

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 and rhodium catalysts.

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

3.5 Carbonylation reactions: Monsanto acetic acid process, olefin hydroformylation- oxo process, carbonylation of alkenes and alkynes in the presence of a nucleophile- the Reppe reaction. Carbonylation of aryl halides in the presence of a nucleophile.

3.6 Olefin methathesis-synthesis gas based reactions, photodehydrogenation catalyst ("Platinum Pop").

3.7 Oxidation of olefins: Palladium catalysed oxidation of ethylene-the Wacker process, epoxidation of olefins, hydroxylation by metal-oxo complexes

3.8 Asymmetric catalysis- Asymmetric hydrogenation, isomerisation and epoxidation.

3.9 C-H activation and functionalization of alkanes and arenes: Radicaltype oxidation, hydroxylation, dehydrogenation, carbonylation and regioselective borylation of alkanes and cycloalkanes. Radical type reactions, electrophilic reactions, carbonylation and borylation of arenes. Insertion of alkenes and alkynes in the Ar-H bond.

3.10 Application of palladium catalysts in the formation of C-O and C-N bonds, oxidative coupling reactions of alkynes with other unsaturated fragments for the formation of cyclic and heterocylic compounds. The Dötz reaction.

Unit 4: Bioinorganic Compounds (18 Hrs)

4.1 Essential and trace elements in biological systems, toxic effects of metals (Cd, Hg, Cr, Pb and As), structure and functions of biological membranes, mechanism of ion transport across membranes, sodium pump, ionophores, valinomycin. Phosphate esters in biology, Redox metalloenzymes, cytochromes-cytochrome P450.

4.2 Oxygen carriers and oxygen transport proteins: Structure and functions of haemoglobins and myoglobin, oxygen transport mechanism, cooperativity, Bohreffect. Structure and functions of haemerythrins and haemocyanin.

4.3 Biochemistry of zinc and copper: Structure and functions of carbonic anhydrase, carboxypeptidase A and superoxide dismutase.

4.4 Other important metal containing biomolecules: Vitamin B_{12} and the vitamin B_{12} coenzymes, photosynthesis-chlorophyll a, PS I and PS II.

4.5 Role of calcium in muscle contraction, blood clotting mechanism and biological calcification. Metals in medicine-therapeutic applications of cis-platin, radioisotopes and MRI agents.

Unit 5: Nuclear Chemistry (9 Hrs)

5.1 Nuclear Reactions: Q value and reaction threshold, reaction cross section, cross section and reaction rate, neutron capture cross section- variation of neutron capture cross section with energy (1/V law). Nuclear fission - fission fragments and mass distribution, fission yields, fission energy, fission cross section and threshold fission neutrons, nuclear fusion reactions and their applications.

5.2 Principles of counting technique: G.M. counter, proportional, ionization and scintillation counters, cloud chamber.

5.3 Synthesis of transuranic elements: Neptunium, Plutonium, Curium, Berkelium, Einsteinium, Mendelevium, Nobelium, Lawrencium

5.4 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.

5.5 Radiation chemistry of water and aqueous solutions. Measurement of radiation doses. Relevance of radiation chemistry in biology, organic compounds and radiation polymerization.

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CH 50 01 02 STRUCTURAL AND MOLECULAR ORGANIC CHEMISTRY

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

Objectives of the Course

To learn and apply the fundamental concepts and mechanisms of organic and photochemical reactions, stereochemistry and conformational analysis of organic compounds.

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

1.1 Review of basic concepts in organic chemistry: Bonding, hybridisation, MO picture of butadiene and allyl systems.

1.2 Electron displacement effects: Inductive effect, electromeric effect, resonance effect, hyperconjugation, steric effect. Bonding weaker than covalent bonds.

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, 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 (9 Hrs)

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

2.2 Catalysis by acids,bases and nucleophiles with examples from acetal, cyanohydrin .Ester formation and hydrolysis reactions of esters-AAC2, AAC1, AAL1, BAC2and BAL1 mechanisms. Hard and soft acids, bases - HSAB principle and its applications (organic reactions only)

Unit 3: Organic Photochemistry (9hrs)

3.1 Photoreactions of carbonyl compounds: Norrish reactions of ketones. Patterno-Buchi reaction. Barton (nitrite ester reaction); Di-π-methane and Photo Fries rearrangements, photochemistry of conjugated dienes (butadiene only), photochemistry of vision.

Unit 4: Stereochemistry of Organic Compounds (18Hrs)

4.1 Stereoisomerism: Definition based on symmetry and energy criteria, configuration and conformational stereoisomers, introduction to Akamppt isomerism(basic idea only)

4.2 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 and threo nomenclature.

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

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

4.5 Geometrical isomerism: nomenclature, E-Z notation, methods of determination of geometrical isomers, interconversion of geometrical isomers.

Unit 5: Conformational Analysis (18 Hrs)

5.1 Conformational descriptors: Factors affecting conformational stability of molecules,conformational analysis of substituted ethanes, cyclohexane and its derivatives, decalins, adamantane, norbornane,sucrose and lactose.

5.2 Conformation and reactivity of elimination (dehalogenation, dehydrohalogenation, semipinacolic deamination and pyrolytic elimination- Saytzeff and Hofmann eliminations),substitution and oxidation of 2^{o} alcohols.

5.3 Chemical consequence of conformational equilibrium - Curtin Hammett principle.

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2. F. A. Carey, R.A. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5^{th} Edn., Springer, 2007.
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13. Nature Chemistry, Vol 10, 2018, pp 618 – 624.

CH 50 01 03 QUANTUM CHEMISTRY AND GROUP THEORY

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

Objective of the course

Revise and update the fundamental ideas, mathematical concepts, applications of group theory and quantum mechanics to molecular systems. The learners should be able to categorise common molecules into various point groups and apply the great orthogonality theorem to derive the character tables of various point groups.

Unit 1: Group Theory and Applications in Chemical Bonding (36 Hrs)

1.1. Symmetry elements and symmetry operations.

1.2. Determination of point groups of molecules and ions (organic / inorganic / complex) belonging to C_n, C_s, C_i, C_{nv}, C_{nh}, $C_{\infty v}$, D_{nh}, $D_{\infty h}$, D_{nd}, T_d and O_h point groups.

1.3. Symmetry in crystals: 32 crystallographic point groups (no derivation), Hermann-Mauguin symbols. Screw axis-pitch and fold of screw axis, glide planes, space groups(elementary idea only)

1.4. Mathematical groups: Properties, Abelian groups, cyclic groups, sub groups, similarity transformation ,classes - C_{2v}, C_{3v} and C_{2h}.

1.5. Group multiplication tables (GMTs) - C_{2v}, C_{3v} and C_{2h}, isomorphic groups.

1.6. Matrix representation of elements like E, Cn, Sn, i, σ-matrix representation of point groups like C_{2v},C_{3v},C_{2h},C_{4v} - trace /character, block factored matrices.

1.7. Reducible and irreducible representations, standard reduction formula, statement of great orthogonality theorem (GOT), construction of character tables for C_{2v}, C_{2h}, C_{3v} and C_{4v}.

1.8. Application in chemical bonding: Projection operator, transformation properties of atomic orbitals, construction of symmetry adapted linear combination of atomic orbitals (SALCs) of C_{2v}, C_{3v}, D_{3h} and C_{2h} molecules.

Unit 2: Quantum Mechanics and Applications (36Hrs)

2.1. Experimental foundation of quantum mechanics: Elementary ideas of black body radiation, photoelectric effect and atomic spectra. Need of quantum mechanics. Concept of matter wave, de Broglie relation, uncertainty principle and its consequences.

2.2. Postulates of Quantum Mechanics: State function or wave function postulate: Born interpretation of the wave function, well behaved functions, orthonormality of wave functions. 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. Eigen value postulate: eigen value equation, eigen functions of commuting operators. Expectation value postulate. Postulate of time-dependent Schrödinger equation, conservative systems and time-independent Schrödinger equation.

2.3. 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.

2.4. 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.

2.5. 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.

2.6. Quantization of angular momentum, quantum mechanical operators corresponding to angular momenta (Lx, Ly, Lz and L^2), commutation relations between these operators. Spherical harmonics as eigen functions of angular momentum operators Lz and L^2. Ladder operator method for angular momentum, space quantization.

2.7. Quantum Mechanics of Hydrogen-like Atoms: 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. Dirac's relativistic equation for hydrogen atom (Elementary idea only).

2.8. Spin orbitals: Construction of spin orbitals from orbitals and spin functions,spin orbitals for many electron atoms, symmetric and antisymmetric wave functions. Pauli's exclusion principle, slater determinants.

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CH 50 01 04THERMODYNAMICS, KINETIC THEORY AND STATISTICALTHERMODYNAMICS

Credit: 4 **Contact Lecture Hours: 54**

Objective of the course

The learners should be able to apply principles and laws of equilibrium thermodynamics to multicomponent systems, to calculate thermodynamic properties of ideal gases and real gases using the principles and techniques of statistical thermodynamics**.** They should be familiar with the properties and theories of gases.

Unit 1: Classical Thermodynamics (18 Hrs)

1.1 Mathematical foundations for thermodynamics-variables of thermodynamics, extensive and intensive quantities, equation for total differential, conversion formulas, exact differentials-general formulation, reciprocity characteristics, homogeneous functions, Euler's theorem.(Non-evaluative)

1.2 Thermodynamic equations of state. Maxwell relations and significance, irreversible processes - Clausius inequality.

1.3 Free energy, thermodynamic equilibria and free energy functions, temperature dependence of free energy - Gibbs Helmholtz equation, applications of Gibbs Helmholtz equation.

1.4 Partial molar quantities, chemical potential and Gibbs-Duhem equations, variation of chemical potential with temperature and pressure, determination of partial molar volume and enthalpy.

1.5 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.

1.6 Thermodynamics of mixing, Gibbs-Duhem-Margules equation, applications of Gibbs-Duhem- Margules equation- Konovalov's first and second laws, excess thermodynamic functions-free energy, enthalpy, entropy and volume, determination of excess enthalpy and volume.

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

1.8 Third law of thermodynamics, Nernst heat theorem, determination of absolute entropies using third law.

1.9 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.

Unit 2: Kinetic Theory of Gases (9 Hrs)

2.1 Derivation of Maxwell's law of distribution of velocities, graphical representation, experimental verification of the law, most probable velocity, derivation of average, RMS and most probable velocities, collision diameter, collision frequency in a single gas and in a mixture of two gases, mean free path, frequency of collision, effusion, the rate of effusion, time dependence of pressure of an effusing gas, the law of corresponding states, transport properties of gases.

Unit 3: Statistical Thermodynamics (27Hrs)

3.1 Brief history about the macroscopic and microscopic approach in science, permutation, probability, Stirling's approximation, macrostates and microstates, equal-apriori principle and thermodynamic probability, phase-space, ensemble, types of ensembles.

3.2 Boltzmann distribution law, partition function and its physical significance, relation between molecular partition function and molar partition function, distinguishable and indistinguishable particles, partition function and thermodynamic functions, separation of partition function-translational, rotational, vibrational, and electronic partition functions, partition function for hydrogen. Thermal de-Broglie wavelength

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

3.4 Need for quantum statistics, Bosons and Fermions, Bose-Einstein statistics:, Bose-Einstein distribution law, Bose-Einstein condensation, first order and higher order phase transitions, liquid helium, Fermi- Dirac statistics:, Fermi- Dirac distribution law, application in electron gas, thermionic emission. Comparison of three statistics.

3.5 Heat capacity of solids- the vibrational properties of solids, Einstein's theory and its limitations, Debye theory and its limitations.

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SEMESTER 2

CH 50 02 01COORDINATION CHEMISTRY

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

Objective of the course

The student shall acquire a foundation of chemistry of sufficient breadth and depth of co-ordination compounds which enable them to understand and apply their knowledge

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^1 and d^9 ions in octahedral and tetrahedral fields (qualitative approach), d-d transitions, selection rules for electronic transitions-effect of spin orbit coupling and vibronic coupling.

2.2 Interpretation of electronic spectra of complexes: Orgel diagrams and demerits, 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 intra molecular interaction, anomalous 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, effect of entering ligand, effect of leaving group and effect of ligands already present on reaction rate, effect of solvent and reaction pathways, substitution in tetrahedral and five-coordinate complexes.

3.2 Kinetics and mechanism of octahedral substitution- water exchange, dissociative and associative mechanisms, base hydrolysis, racemization reactions, solvolytic reactions (acidic and basic). Replacement reactions involving multidendate ligands- formation of chelates, effect of H^+ on the rates of substitution of chelate complexes, metal ion assisted and ligand assisted dechelation.

3.3 Electron transfer reactions: Outer sphere mechanism-Marcus theory, inner sphere mechanism-Taube mechanism, mixed outer and inner sphere reactions, two electron transfer and intramolecular electron transfer.

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 Lanthanoids and Actinoids (9 Hrs)

5.1 Term symbols for lanthanide ions, inorganic compounds and coordination complexes of the lanthanoids upto coordination No.12, electronic spectra and magnetic properties of lanthanoid complexes,organometallic complexes of the lanthanoids- σ-bonded complexes, cyclopentadienyl complexes, organolanthanoid complexes as catalysts.

5.2 General characteristics of actinoids-difference between 4f and 5f orbitals, coordination complexes of the actinoids- sandwich complexes, coordination complexes and organometallic compounds of thorium and uranium, comparative account of coordination chemistry of lanthanoids and actinoids with special reference to electronic spectra and magnetic properties.

References

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

2. J. E. Huheey, E. A. Keiter, R. A. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Pearson Education India, 2006.
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8. J. D. Lee, Concise Inorganic Chemistry, 4th Edn., Wiley-India, 2008
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11. C. E. Housecroft, A. G. Sharpe, Inorganic Chemistry, Pearson, 2012.

CH 50 02 02 ORGANIC REACTION MECHANISMS

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

Objective of the course

To learn and understand the involvement of reactive intermediates, their structure and reactivity through various organic reactions, the orbital interactions (Woodward Hoffmann rules) in concerted reactions and apply knowledge for solving problems.

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), 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: Name 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 sulphurylids - 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 Reactions of carbenes such as Wolff rearrangement, Reimer-Tiemannreaction. Reactions of ylides 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 and intramolecular) for C-C bond formation - Baldwin's rules (b) fragmentation and rearrangements - Hydroperoxide: formation, rearrangement and reactions. Autooxidation.

5.2 Name 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, Aldol condensation, 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,ene and dyotropic reactions. Woodward Hoffmann rules - Frontier orbital and orbital symmetry correlation approaches - PMO method (for electrocyclic and cycloaddition reactions only).

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 (Cope reaction), Acetates and Xanthates (Chugaeve reaction).

7.4 Problems based on the above topics

References

1. R. Bruckner, Advanced Organic Chemistry: Reaction Mechanism, Academic Press, 2002.
2. F. A. Carey, R.A. Sundberg, Advanced Organic Chemistry, Part B: Reactions and Synthesis, 5th Edn., Springer, 2007.
3. W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, Cambridge University Press, 2005.
4. J. March, M.B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6th Edn., Wiley, 2007.
5. A. Fleming, Frontier Orbitals and Organic Chemical Reactions, Wiley, 1976.
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CH 50 02 03 CHEMICAL BONDING AND COMPUTATIONAL CHEMISTRY

Credit: 3 **Contact Lecture Hours: 72**

Objective of the course

The learners should be able to apply, analyze and evaluate group theoretical concepts in spectroscopy, extent the ideas of quantum mechanics from one electron system to many electron systems and various theories of chemical bonding.

Unit 1: Application of Group Theory in Spectroscopy (18hrs)

1.1. Vibrational mode analysis using group theory taking H_2O, NH_3 and trans-N_2F_2 as examples using symmetry coordinates and internal coordinates method, prediction of IR and Raman activity, rule of mutual exclusion, redundant modes, out of plane modes.

1.2. Application in uv-visible spectroscopy, selection rules, orbital selection rules, transitions between non-degenerate states, prediction of electronic transitions in C_{2v},C_{3v},C_{4v},C_{2h} and C_{4h} using direct product terms , spin selection rules, relaxation in selection rules and distortion .

1.3. Application in hybridization, determination of hybridization and hybrid functions in CH_4, BF_3 and PCl_5

1.4. Group theory and optical activity(brief study)

Unit 2: Approximation Methods in Quantum Mechanics (18 Hrs)

2.1 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 $e^{-\alpha r}$ for the hydrogen atom, variation treatment for the ground state of helium atom.

2.2 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.

2.3 Hartree-Fock method, multi-electron atoms. Hartree-Fock equations (no derivation). The Fock operator, core hamiltonian, coulomb operator and exchange operator. 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 3: Chemical Bonding **(18 Hrs)**

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

3.2 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.

3.3 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 4: Computational Quantum Chemistry **(18 Hrs)**

4.1 Introduction and scope of computational chemistry, potential energy surface, conformational search, global minimum, local minima, saddle points.

4.2 Ab initio methods: A review of Hartee-Fock method, self-consistent field (SCF) procedure. Roothan concept basis functions. Basis sets and its classification: Slater type and Gaussian type basis sets, minimal basis set, Pople style basis sets . Hartree-Fock limit. Post Hartree-Fock methods - introduction to Møller Plesset perturbation theory, configuration interaction, coupled cluster and semi empirical methods.

4.3 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).

4.4 Comparison of ab initio, semi empirical and DFT methods.

4.5 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 and ethane. General format of GAMESS / Firefly input file , single point energy calculation, geometry optimization, constrained optimization and frequency calculation. Koopmans' theorem.

4.6 Features of molecular mechanics force field-bond stretching, angle bending, torsional terms, non-bonded interactions and electrostatic interactions. Commonly used force fields- AMBER and CHARMM.

References

1. N. Levine, Quantum Chemistry, 7th Edn., Pearson Education Inc., 2016.
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18. K.I. Ramachandran, G. Deepa, K. Namboori, Computational Chemistry and Molecular Modeling: Principles and Applications, Springer, 2008.
19. A. Hinchliffe, Molecular Modelling for Beginners, 2nd Edn., John Wiley & Sons, 2008.
20. C.J. Cramer, Essentials of Computational Chemistry: Theories and Models, 2nd Edn., John Wiley & Sons, 2004.
21. D.C. Young, Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems, John Wiley & Sons, 2001.

Softwares:

a. Molecular Mechanics: Arguslab, Tinker, NAMD, Tinker, DL-POLY, CHARMM, AMBER
b. Firefly / PC GAMESS available from http://classic.chem.msu.su/gran/gamess/
c. WINGAMESS available from http://www.msg.ameslab.gov/gamess/ Graphical User nterface (GUI):
d. Gabedit available from http://gabedit.sourceforge.net/
e. wxMacMolPlt available from http://www.scl.ameslab.gov/MacMolPlt/

CH 50 02 04 MOLECULAR SPECTROSCOPY

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

Objective of the course

To learn basic principles and theory of microwave, NMR, IR, Raman, UV-Vis spectroscopy.

Unit 1: Foundations of Spectroscopic Techniques (3 Hrs)

1.1. Regions of the electromagnetic radiation, origin of spectrum, intensity of absorption, signal to noise ratio, natural line width. Doppler broadening, Lamb dip spectrum, Born Oppenheimer approximation.

Unit 2: Microwave Spectroscopy (6 Hrs)

2.1 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.

2.2 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.

Unit 3: Infrared and Raman Spectroscopy (9 Hrs)

3.1 Morse potential energy diagram, fundamental vibrations, overtones and hot bands, determination of force constants, diatomic vibrating rotator, break down of the Born-Oppenheimer approximation, effect of nuclear spin.

3.2 Vibrational spectra of polyatomic molecules, normal modes of vibrations, combination and difference bands, Fermi resonance. FT technique, introduction to FTIR spectroscopy. Instrumentation of FTIR

3.3 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.

Unit 4: Electronic Spectroscopy (9 Hrs)

4.1 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.

4.2 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.

Unit 5: Nuclear Magnetic Resonance Spectroscopy (18 Hrs)

5.1 Theory of NMR Spectroscopy: Interaction between nuclear spin and applied magnetic field, important magnetically active nuclei. Nuclear energy levels, population of energy levels, Larmor precession, relaxation methods. Chemical shift and its representation- δ scale of PMR and CMR. Spin-spin coupling: Theory and illustration with AX system.

5.2 Fourier Transformation (FT) NMR Spectroscopy: Instrumentation of NMR technique, magnets, probe and probe tuning, Creating NMR signals, effect of pulses, rotating frame reference, FID, FT technique, data acquisition and storage. Pulse sequences-Pulse width, spins and magnetisation vector.

5.3 Solid state NMR-Applications. Magic Angle Spinning(MAS).

Unit 6: Other Magnetic Resonance Techniques (9 Hrs)

6.1 EPR Spectroscopy: Electron spin in molecules, interaction with magnetic field, g factor, factors affecting g values, determination of g values ($g_{||}$ and $g^{\perp}$), fine structure and hyperfine structure, Kramers' degeneracy, McConnell equation.

6.2 Theory and important applications of NQR Spectroscopy.

6.3 Mossbauer Spectroscopy: Principle, Doppler effect, recording of spectrum, chemical shift, factors determining chemical shift, application to metal complexes.

References

1. C. N. Banwell, E. M. McCash, Fundamentals of Molecular Spectroscopy, 4th Edn., Tata McGraw Hill, 1994.
2. G. Aruldhas, Molecular Structure and Spectroscopy, Prentice Hall of India, 2001.
3. A. U. Rahman, M.I. Choudhary, Solving Problems with NMR Spectroscopy, Academic Press, 1996.
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SEMESTERS 1 AND 2

CH 50 02 05 INORGANIC CHEMISTRY PRACTICAL-1

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

Objective of the Course

The learners should be able to apply the principles of qualitative and quantitative analytical techniques in inorganic chemistry for identification of ions and preparation and characterization of inorganic complexes

PART I

Separation and identification of a mixture of four cations (a mixture of two familiar ions such as Ag^{+} , Hg^{2+}, Pb^{2+}, Cu^{2+}, Bi^{2+}, Cd^{2+}, As^{3+}, $Sn^{2+,}$ Sb^{3+}, Fe^{2+}, Fe^{3+}, Al^{3+}, Cr^{3+}, Zn^{2+} , Mn^{2+}, Co2+, Ni^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}, Mg^{2+}, Li^{+} , Na^{+} , K^{+} and $NH4^{+}$ and 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, NH4+, 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.

(f) Bis(dimethylglyoximato)nickel(II)

(g) Prussian blue

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1. A.I. Vogel, G. Svehla, Vogel's Qualitative Inorganic Analysis, 7th Edn., Longman,1996.
2. A.I. Vogel, A Text Book of Quantitative Inorganic Analysis, Longman, 1966.
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CH 50 02 06 ORGANIC CHEMISTRY PRACTICAL-1

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

Objective of the Course

The learners should be able to apply class room learning separation and purification of organic compounds and binary mixtures. They should be able to use the computational tools to draw the reaction schemes and spectral data to various organic reactions

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. Quantitative separation of organic mixtures by column chromatography – Purity assessment of the components by TLC.

PART III

Drawing the reaction schemes (Based on Semester 1 and 2 theory) 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. Condensation
(a) Dieckmann condensation
(b) Claisen condensation
(c) Darzen condensation
(d) Aldol condensation
2. Oxidation / Reduction
(a) Ozonolysis
(b) Baeyer Villiger oxidation
(c) Cannizaro reaction
(d) Clemmenson reduction
3. Rearrangement
(a) Benzilic acid rearrangement
(b) Pinacol – Pinacolone rearrangement
(c) Dienone – Phenol rearrangement
(d) Wagner – Meerwein rearrangement

4. Pericyclic reaction

(a) Diels – Alder reaction

(b) Cope rearrangement

References

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CH 50 02 07 PHYSICAL CHEMISTRY PRACTICAL-1.

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

Objective of the Course

The learners should be able to apply the conceptual understanding acquired from the theory classes

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

PART A

I. Adsorption

Verification of Freundlich and Langmuir adsorption isotherm Charcoal Acetic acid or Charcoal-Oxalic acid system

Determination of concentration of given acid using the isotherm

II. Phase diagrams

Construction of phase diagram of simple eutectics

Effect of KCl/Succinic acid on Critical Solution Temperature of phenol water system

Construction of phase diagram of three component system with one pair of partially miscible liquids

III. Distribution law

Distribution coefficient of Iodine between an organic solvent and water

Determination of the equilibrium constant of the reaction $KI+I_2 \rightarrow KI_3$

Determination of unknown concentration of KI

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
4. Determination of CMC of surfactants by surface tension measurements

V. Determination of heat of solution from solubility measurements

PART B

Computational chemistry experiments

VI. Experiments illustrating the capabilities of modern open source/ free computational chemistry packages in computing.

(a) Single point energy

(b) Geometry optimization

(c) Vibrational frequencies

(d) Population analysis

(e) Conformational analysis of ethane, transition state search

(f) Molecular orbitals, ionisation energy, electron affinity

(g) Dipolemoment, freevalence, bond order

(h) Determination of inversion barrier of simple molecules like NH_3 , H_2O, H_2O_2

(I) Determination of Z-matrices /Cartesian coordinates of furan, thiophene, pyrrole and benzene using structure drawing programs like Chemsketch and wwMacMolPlt.

References

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3. J.H. Jensen, Molecular Modeling Basics, CRC Press, 2010.
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SEMESTER 3

CH 50 03 01 STRUCTURAL INORGANIC CHEMISTRY

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

Objective of the Course

The students must acquire basic information about the imperfections of solids, electrical and magnetic properties of solidsand properties of inorganic chains, rings, cages and clusters. They should have awareness about organometallic polymers and magnetic nanoparticles.

Unit 1: Solid State Chemistry (18 Hrs)

1.1 Structure of solids: Imperfections in solids- line defects and plane defects. Structure of the following compounds - Zinc blende, Wurtzite, Rutile, fluorite, antifluorite, Nickel Arsenide, Perosvskite and 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 vapour deposition technique.

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

2.1 Free electron theory of solids. Band theory of solids: Applications to Transition metal compounds and compounds like NaCl, MgO and fullerenes. Energy bands-conductors and non-conductors, Mechanism of intrinsic and extrinsic semiconductors. Mobility of charge carriers- Hall Effect (derivation required). Piezo electricity, pyroelectricity and ferro electricity- hysteresis.

2.2 Magnetic properties of transition metal oxides, garnets, spinels, ilmenites and perovskites, magnetoplumbites. Photoconductivity, photovoltaic effects, luminescence,applications of optical properties-phosphors, solid state lasers and solar cells.

2.4 Conductivity of pure metals. Super conductivity-Type I and Type II superconductors, Meisner effect, BCS theory of superconductivity (derivation not required)-Cooper pairs. High temperature superconductors, super conducting cuprates - YBaCu oxide system. Josephson's Junction, conventional superconductors, organic superconductors, fullerenes, carbon nanotubes and graphenes.

Unit 3: Inorganic Chains and Rings (9 Hrs)

3.1 Chains: Catenation, heterocatenation, silicones. Zeolites: Synthesis, structure and applications, isopoly acids of vanadium, molybdenum and tungsten, heteropoly acids of Mo and W, polythiazil-one dimensional conductors. Infinite metal chains

3.2 Rings, topological approach to boron hydrides, styx numbers. 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 Clusters (9 Hrs)

4.1 Synthesis, structure and bonding of cage like structures of phosphorous. Boron cage Aluminium, indium and gallium clusters, cages and clusters of germanium, tin and lead, cages and clusters of tellurium, Mercuride clusters in amalgams. Medical applications of boron clusters- nucleic acid precursors, DNA binders, application of C_2B_{10} for Drug Design, Nuclear receptor ligands bearing C_2B_{10}cages.

Unit 5: Organometallic Polymers (9 Hrs)

5.1 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, poly(ferrocenylsilane)s, applications of Poly(ferrocenylsilane)s and related polymers, applications of rigid-rod polyynes, polygermanes and polystannanes, polymers prepared by ring opening polymerization, organometallic dendrimers.

Unit 6: Magnetic Nanoparticles and Synthesis of Solids (9 Hrs)

6.1 Synthesis of Solids: Nucleation, growth, epitaxy and topotaxy,methods for the synthesis of $MgAl_2O_4$, silica glass, indium tin oxide and their coatings, zeolites and alumina based abrasives, hydrothermal synthesis, intercalation and deintercalation,preparation of thin films, electrochemical methods, chemical vapour deposition. Synthesis of amorphous silica and diamond films, sputtering and laser ablation.

6.2 Magnetic nanoparticles, superparamagnetism and thin films, applications of magnetic nanoparticles- data storage, Magnetic Resonance Imaging (MRI) and Contrast Enhancement using magnetic nanoparticles, biomedical applications of magnetic nanoparticles.

References

1. L.V. Azaroff, Introduction to Solids, Mc Graw Hill, 1984.
2. A.R. West, Solid State Chemistry and its Applications, Wiley-India, 2007.
3. D.K. Chakrabarty, Solid State Chemistry, New Age Pub., 2010.

4. D.M. Adams, Inorganic Solids: An Introduction to Concepts in Solid State Structural Chemistry, Wiley, 1974.
5. C.N.R. Rao, K.J. Rao, Phase Transitions in Solids, McGraw Hill, 2010.
6. B.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., John Wiley & sons, 2006.
7. A. Earnshaw, Introduction to Magnetochemistry, Academic Press, 1968.
8. J.E. Huheey, E.A. Keiter, R.L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Harper Collins College Pub.,1993.
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12. Matthias Driess, Heinrich Nöth, Molecular Clusters of the Main Group Elements, Wiley-VCH, 2004.
13. Richard J.D. Tilley, Understanding Solids, 2nd edition, Wiley, 2013.
14. G.L. Hornyak, J.J. Moore, H.F. Tibbals, J. Dutta, Fundamentals of Nanotechnology, CRC Press, 2009.
15. Chris Binns, Introduction to nanoscience and nanotechnology, wiley, 2010.
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17. Anthony R. West, Basic Solid State Chemistry, John Wiley and Sons, 1988.

CH 05 03 02 CHEMICAL KINETICS AND SURFACE 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 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 Steady state approximation-chain reactions, H_2-Br_2 reaction, H_2-Cl_2 reaction.

1.3 Reactions in solution: Factors determining reaction rates in solutions-cage effect, effect of dielectric constant and ionic strength, Bronsted-Bjerrum equation, primary and secondary kinetic salt effect, influence of solvent on reaction rates, kinetic isotope effects.

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

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

1.6 Enzyme catalysis and its mechanism, Michelis-Menten equation, Lineweaver-Burk method, effect of pH and temperature on enzyme catalysis.

1.7 Introduction to oscillating chemical reactions: Lotka-Voltera model, molecular interactions in molecular beams-basic principles, the differential scattering cross-section, the phenomena of glory scattering and rainbow scattering.

Unit 2: Surface Chemistry and Colloids (18 Hrs)

2.1 Adsorption: Gibbs adsorption equation and its verification, 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, Eley-Rideal mechanism, Langmuir-Hinshelwood mechanism.

2.2 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.

2.3 Surface Enhanced Raman Scattering, surfaces for SERS studies, chemical enhancement mechanism, surface selection rules, spectrum of 2-aminophenol, applications of SERS.

2.4 Colloids: Zeta potential, electro kinetic phenomena, sedimentation potential and streaming potential, Donnan membrane equilibrium.

Unit 3: Advanced Thermodynamics (9 Hrs)

3.1 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, Onsager reciprocal relations, thermal osmosis, thermoelectric phenomena.

3.2 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 4: Photochemistry (9 Hrs)

4.1 Quantum yield, chemical actinometry, photosensitization, chemiluminescence, bioluminescence, thermoluminescence, pulse radiolysis, hydrated electrons, photostationary state, dimerisation of anthracene, ozone layer in the atmosphere, chemistry of photosynthesis.

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

4.3 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, greenhouse effect, application of pulsed laser in measuring the dynamics of photochemical processes, photochemistry of vision.

Unit 5: Electro and Thermo analytical Techniques (9 Hrs)

5.1 Amperometric titrations: General principles of amperometry, application of amperometry in the qualitative analysis of anions and cations in solution, titration procedure, merits and demerits of amperometric titrations.

5.2 Coulometry: Coulometer-Hydrogen Oxygen coulometers, silver coulometer, coulometric analysis with constant current, coulometric titrations, application of coulometric titrations-neutralization titrations, complex formation titrations, redox titrations, advantages of coulometry.

5.3 Differential Thermal analysis (DTA): Principle, instrumentation, advantages and disadvantages, Pharmaceutical applications, derivative differential thermal analysis (DDTA), TGA-principle, instrumentation, factors affecting results, advantages and disadvantages, pharmaceutical applications.

Unit 6: Nano Science (9 Hrs)

6.1 Nanochemistry: Synthesis-bottom up and top down methods-physical vapour deposition, CVD, precipitation, sol-gel, microemulsion methods.

6.2 Classification: quantum dots, one dimensional and two dimensional nanostructures.

6.3 Properties: Optical, electrical and magnetic properties.

6.4 Characterizations: X-ray, XPS, UV, SEM, TEM.

6.5 Applications of nano materials in catalysis, lithography, photonics and medicine.

References

1. J. Rajaram, J. C. Kuriakose, Kinetics and Mechanisms of Chemical Transformations, Macmillan India, 2000.
2. K. J. Laidler, Chemical Kinetics, 3rd Edn., Harper & Row, 1987.
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11. D. A. Skoog, D. M. West, F. J. Holler, S. R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College Pub., 2007.
12. A.I. Vogel, A Text Book of Quantitative Analysis including Instrumental Analysis, John Wiley & Sons, 1961.
13. Charles, P., Poole Jr., Frank J. Owens, Introduction to Nano Technology, 2009.
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CH 05 03 03 CONCEPTS OF POLYMER CHEMISTRY

Credit: 4 **Contact Lecture hours 72**

Unit 1: Introduction to Polymer Chemistry (9 Hrs)

1.1 Nomenclature of polymers: Nomenclature based on source and structure (Non-IUPAC), IUPAC structure-based nomenclature system, trade names.

1.2 Classification, the rise of macromolecular science, industrial scenario, molecular forces and chemical bonding in polymers.

1.3 Basic terms and definitions: Monomer, polymer, end groups, degree of polymerisation, copolymers, average molecular weight and distribution, polymer morphology, thermoplastics, elastomers, plastics, thermosetting resin, polymer blends.

Unit 2: Polymer Reactions and Polymeric Reagents (18 Hrs)

2.1 Principles of polymer reactivity: Yield, isolation of functional groups, concentration, crystallinity, change in solubility, crosslinking, steric effects, electrostatic effects, neighbouring-group effects, hydrophobic interactions.

2.2 Crosslinking: Alkyds, elastomers based on 1, 3-dienes-sulfur alone, accelerated sulfur vulcanization, peroxide and radiation crosslinking.

2.3 Reactions of cellulose: Dissolution, esterification and etherification.

2.4 Graft copolymers: Radical graft polymerization-vinyl macromonomers, chain transfer and copolymerization, ionizing radiation, redox initiation, living radical polymerization, anionic graft polymerization, cationic graft polymerization.

2.5 Miscellaneous polymer reactions: Halogenation-natural rubber, saturated hydrocarbon polymers. Aromatic substitution, cyclisation, reactions of poly(vinyl acetate).

2.6 Polymer supported reagents: Oxidising reagents, reducing reagents, bases, coupling reagents, catalysts, wittig reagents, polymer supports in solid phase peptide and protein synthesis.

Unit 3: Special Methods for Polymer Synthesis (9 Hrs)

3.1 Metathesis, group-transfer polymerisation, macromers in polymer synthesis, genetic engineering, solid state-gas phase-plasma polymerisation, polymerisation in supercritical fluids, polymerisation in ionic liquids, click chemistry for polymerisation, Ziegler Natta polymerizations.

Unit 4: Polymerisation Mechanisms and Polymerisation Techniques (18 Hrs)

4.1 Step-reaction (condensation) polymerisation: Mechanism, kinetics, linear stepwise polymerization, polyfunctional step-reaction polymerization.

4.2 Radical chain(addition) polymerization: Mechanism of vinyl polymerization, kinetics of vinyl radical polymerization, effects of temperature and pressure on chain polymerization.

4.3 Living radical polymerization: Atom transfer radical polymerization(ATRP), stable free-radical polymerisation(SFRP), radical addition-fragmentation transfer (RAFT).

4.4 Ionic and coordination chain(addition) polymerization: Cationic polymerization, anionic polymerization, coordination polymerization.

4.5 Copolymerisation: Kinetics, composition of copolymers, mechanism, block and graft copolymers.

4.6 Ring opening polymerization: Poly(propylene oxide), epoxy resins, polycaprolactam (nylon 6)

4.7 Polymerisation techniques: Bulk polymerization, solution polymerization, suspension polymerization, emulsion polymerization.

Unit 5: Stereochemistry of Polymers (18 Hrs)

5.1 Basic definitions: Configurational unit, configurational base unit, configurational repeating unit, stereorepeating unit, tacticity, isotactic polymer, syndiotactic polymer, stereoregular polymer, atactic polymer, stereospecific polymerisation, cistactic polymer, transtactic polymer, block, tactic block polymer, stereoblock polymer.

5.2 Stereoisomerism in polymers: Monosubstituted ethylene-site of steric isomerism, tacticity. Disubstituted ethylenes- 1,1-disubstituted ethylene, 1,2-disubstituted ethylene, carbonyl and ring opening polymerisation.

5.3 Properties of stereoregular polymers: Significance of stereoregularity, isotactic, syndiotactic, and atactic polypropenes, *cis*- and *trans*-1,4-poly-1,3-dienes, cellulose and amylose, analysis of stereoregularity.

5.4 Optical activity in polymers: Optically active monomers, chiral conformation, enantiomer-differentiating polymerisation, asymmetric induction.

5.5 Chain conformations: Trans-gauche conformations, steric effects, conformations of poly ethylene.

References

1. Fred W. Billmeyer Jr., A Textbook of Polymer Science, 3rd Edn., 1984.
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CH 50 03 04 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-applications.

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 1H and 13C 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- Dirac model. Karplus curve, quadrupole broadening and decoupling, homotopic, enantiotopic and diastereotopic protons, virtual coupling, long range coupling. 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. 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-TOF, PD, Field Desorption Electrospray Ionization. Fragmentation patterns (polyenes, alkyl halides, alcohols, phenols, aldehydes and ketones, esters). 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, 1H NMR and 13C 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.

5.3 Spectral analysis of the following reactions/functional transformations:

a. Pinacol-Pinacolone rearrangement
b. Benzoin condensation
c. (4+2) cycloaddition
d. Beckmann rearrangement
e. Cis-trans isomerisation of azo compounds
f. Benzil-benzilic acid rearrangement
g. Fries rearrangement

References

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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 one group of 3 courses to be opted from the following two groups)

GROUP A ELECTIVE COURSES

CH 88 04 01 PROPERTIES AND CHARACTERISATION METHODS OF POLYMERS

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

Unit 1: Morphology and Order in Crystalline Polymers (18 Hrs)

1.1 Polymer morphology: Common polymer morphologies, structural requirements for crystallinity, degree of crystallinity, crystallisability-mechanism of crystallisation.

1.2 Polymer single crystals: Lamellae, complex structures, disorder and nature of the fold surfaces.

1.3 Structure of polymers crystallized from melt: The fringed micelle concept, the defect structure of crystalline polymers, extended-chain crystals, structure of spherulites, relation of sherulites to crystallites, morphology of sperulites.

1.4 Theory of crystallisation: Avrami equation, Hoffman's nucleation theory, the entropic barrier theory.

1.5 Strain induced morphology: Fibrillar crystallisation, cold drawing, morphology changes during orientation, degree of orientation-X-ray diffraction, birefringes, infrared dichroism.

1.6 Morphological analysis: Optical microscopy, electron microscopy (SEM and TEM), atomic force microscopy.

Unit 2: Polymer Solutions (18 Hrs)

2.1 Criteria for polymer solubility: Solubility, polymer texture and solubility, the concept of solubility parameter, Hildebrand solubility parameter and its application.

2.2 Thermodynamics of polymer solution: Flory-Huggins theory(liquid lattice theory), modified Flory-Huggins theory, entropy of mixing, enthalpy and free energy of mixing, dilute polymer solutions (Flory-Krigbaum theory), advantages and limitation of FH and FK theories, corresponding state theories.

2.3 Phase Equilibrium: Polymer-solvent miscibility, binary polymer-solvent systems, ternary systems, multicomponent systems, polymer-polymer miscibility,

2.4 Fractionation of polymers by solubility: Bulk fractionation by nonsolvent addition, column elution-solvent gradient elution, thermal gradient elution, analytical precipitation techniques-summative fractionation, turbidimetric titration.

2.5 Conformations of polymer chain in solution: End-to-end dimension, the freely joined chain, real polymer chains, fixed bond angle-freely rotating, fixed bond angle-restricted rotation, long range interactions.

Unit 3: Properties and Testing of Polymers (27 Hrs)

3.1 Testing: Overview of various testing methods and standards such as ASTM, BIS and ISO. Test specimen preparation-milling, punching, template, cutting from sheets or films product.

3.2 Mechanical properties of polymers: Stress-strain properties in tension, tensile strength, fatigue tests, flexural strength, impact tests, tear resistance, hardness, abrasion resistance, creep and stress relaxation, dynamic mechanical analysis (DMA), Young's modulus, polymer fracture behaviour-brittle fracture, linear elastic fracture mechanics. Hardness test methods- principle of hardness testing, conventional hardness testing methods, test methods for determining hardness values after unloading, test methods for determining hardness values under load, comparability of hardness values, instrumented hardness test-fundamentals of measurement methodology, material parameters derived from instrumented hardness tests. Quasi-static test methods-deformation behaviour of polymers, tensile tests on polymers-theoretical basis of the tensile test, conventional tensile tests, enhanced information of tensile tests, tear test, compression test on polymers-theoretical basis of the compression test, performance and evaluation of compression tests, bend tests on polymers-theoretical basis of the bend best.

3.3 Thermal properties: Thermal conductivity, thermal expansion, heat capacity, heat deflection temperature, vicat softening temperature, torsion pendulum test, glass transition temperature.

3.4 Electrical properties: Dielectric strength, short time method, slow rate of rise method, step by step method, dielectric constant and dissipation factor, arc resistance test. Conducting polymers-conduction mechanism, applications of conducting polymers with examples, polymers with piezo, pyro, ferro electric characters.

3.5 Optical properties: transmittance and reflectance, gloss, haze, transparency, refractive index.

3.6 Polymer viscoelasticity: Introduction, simple rheological responses-the ideal elastic response, pure viscous flow, rubberlike elastic, viscoelasticity-mechanical models for linear viscoelastic response, Maxwell model-creep experiment, stress relaxation experiment, dynamic experiment, the Voight element, the four-parameter model, material response time-the Deborah Number, relaxation and retardation

spectra, Maxwell-Weichert model (relaxation), Voight-Kelvin (creep) model, superposition principle-Boltzmann superposition principle, time-temperature superposition principle.

Unit 4: Characterisation Methods of Polymers (18 Hrs)

4.1 Polymer molecular weight characterization: Molecular weight distribution, number average molecular weight determination-osmometry techniques, end group analysis, colligative property measurements. Weight average molecular weight determination-light scattering technique, sedimentation technique, higher average molecular weight determination-gel permeation chromatography (GPC), viscosity average molecular weight (Mŋ) determination-viscometry, ultracentrifugation.

4.2 Spectroscopic methods of characterization: Vibrational spectroscopy methods-IR, Raman spectroscopy. Resonance method-NMR spectroscopy, diffusion-ordered NMR spectroscopy (DOSY). Electronic spectroscopy methods- UV/visible spectroscopy, fluorescence, electron spin resonance (ESR). Scattering spectroscopy methods-X-ray diffraction, X-ray crystallography, small angle neutron scattering. Mass spectroscopy method characterization, molecular relaxation spectroscopy-X-ray and neutron scattering methods.

4.3 Microscopy methods: Transmission electron microscopy (TEM), scanning electron microscopy (SEM).

4.4 Thermo-analytical methods: Differential scanning calorimetry (DSC), differential thermal analysis (DTA), thermo-mechanical analysis, thermo-gravimetric analysis.

Unit 5: Polymer Waste Management (9 Hrs)

5.1 Analysis of polymer wastes: Flouresence labelling, time-gated fluorescence spectroscopy, identification of black plastics, life cycle assessment, analysis of contaminated mixed waste plastics, application of Raman spectroscopy in waste analysis, SPI codes.

5.2 Management: Source reduction, product reuse, durable products, recycling of plastic wastes, plastic waste to energy, landfilling of waste plastics, alternative plastic materials.

5.3 Polymer recycling: Recycling codes, mechanical recycling-primary and secondary, chemical recycling-tertiary recycling, quaternary recycling- thermal utilisation, renewable polymer synthesis, sustainable bio-plastic production through landfill methane recycling.

5.4 Biodegradable polymers, degradation products in degradable polymers, recycling BIOPOL-composting, laboratory-scale composting, test methods to determine

polymer biodegradability, synthesis and applications of photodegradable poly (ethylene terephthalate).

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1. Fred W. Billmeyer Jr. Textbook of Polymer Science, 3rd Edn., John Wiley & Sons, Asia, 1994.
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CH 88 04 02 ADVANCES IN POLYMER SCIENCE AND TECHNOLOGY

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

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

1.1 Poly electrolytes-water soluble charged polymers, ionomers (ion containing polymers), conducting polymers, solid polymer electrolytes (SPE), electroluminescent polymers, fluoropolymers, block copolymers(multiphase polymers), polymer colloids, thermoplastic elastomers(TPE), polyblends (heterogeneous plastics), inter penetrating network (IPN) polymers, thermally stable polymers, telechelic polymers (functional polymers) polymer microgel, biomedical polymers.

1.2 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, application of liquid crystalline polymers.

1.3 Dendritic polymers: Origin of dendrimers, structure, properties, design and synthesis-divergent growth method, convergent growth method, medicinal application.

1.4 Introduction to: Polymers for organic light-emitting diodes (OLEDs), organic and hybrid solar cell, supramolecular polymer science.

Unit 2: Adhesives and Surface Coating **(9 Hrs)**

2.1 Adhesives: Introduction, theory, surface treatment, joint design, physical nature of adhesives, types of adhesives, natural glues, applications, elastomer adhesives, synthetic adhesives, olefinic polymer adhesives, types of epoxy adhesives, inorganic adhesives, bio adhesives, test methods in determining the strength and properties of adhesives.

2.2 Surface coating: Introduction, types of coating, drying oils, types of resins, surfactants, surface preparation, solvent selection, methods of coating, theory of powder coating, application of powder coating, curving process. Corrosion, electroplating, hazards and safety measures in paint industry.

Unit 3: Polymer Blends and Composites **(18 Hrs)**

3.1 Polymer blends: Classification, principles and methods involved in the preparation of different polymer blends, study of polymer blends and alloys on the basis of miscibility, criteria for selection of polymer. Compatibility of blends-principles of solubility and compatibility, thermodynamics of miscibility, mechanical compatibility. Phase morphology-Phase separation behaviour, morphology of blends and its determination- electron microscopy- domain structure.

3.2 Introduction to rheology of polymer blends: Relevance in processing, rheology–phase morphology relationships and their relevance, micro rheology, rheological models-solution, and suspension models.

3.3 Industrial applications of polymer blends.

3.4 Polymer composites: Fundamental concepts, factors influencing the performance of polymer composites-aspect ratio, void content, length of the fibre, nature of the fibre. Structure property relationship between fibre and matrix, modifications of the fibre surface, degree of interaction between fibre and matrix, wetting behaviour, degree of cross linking etc.,

3.5 Processing of thermoplastic composites: Types of processing methods, solution, film, lamination, sandwich etc., processing conditions, advantages and disadvantages.

3.6 Fabrications of thermoset composites: Hand layup method, compression and transfer moulding, pressure and vacuum bag process, filament winding, protrusion, reinforced RIM, RRIM, injection moulding of thermosets, SMC and DMC.

3.7 Nano-composites: Definition, types, methods of fabrication, characterization. Polymer/CNTs and Polymer/Nanoclay based composites, properties and their functional applications.

Unit 4: Polymer Compounding and Processing (18 Hrs)

4.1 Polymer mixing: Introduction, basic concepts, mechanism of mixing and dispersion, mixing of solid-solid, liquid-liquid and liquid-solid, dispersive mixing, distributive mixing and laminar mixing, mixing indices, kinetics of mixing, rheology of filled polymers.

4.2 Compounding: Introduction, types and characteristics of compounds-polymer blends, polymer formulations, filled polymers and polymer composites, compounding practice, mixing types, solid additives, morphology of filler additives, compatibilizers-mechanism and theory, filler surface modification and interfacial agents, dispersion of polymer nanoparticles in polymer melt, fillers and reinforcements *viz.* carbon black, ZnO, calcium carbonate, titanium oxide, nano clay, glass fibers, organic fillers, nanofillers. Compounding ingredients for rubber-fillers, reinforcing, semi reinforcing and nonreinforcing, 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.

4.3 Polymer processing: Casting-die casting, rotational casting, film casting, thermoforming, foaming, lamination, reinforcing, processing of fibres-dry spinning, wet spinning, melt spinning, moulding processes-compression moulding, injection moulding, transfer moulding, blow moulding, extrusion moulding, calendaring.

Unit 5: Fibre Science and Technology (9 Hrs)

5.1 Basic concepts, structural attributes of fibres, fibre characteristics.

5.2 Natural fibres: Natural fibres of vegetable origin, the seed and fruit fibres, natural fibres of animal origin-silk, natural mineral fibre.

5.3 Man-made fibres: Introduction, spinning, semi-synthetic fibres from cellulose, regenerated protein fibres, synthetic fibres-rayon, polyethylene terephthalate, nylon 6 and nylon 66, polyolefins, polyvinyl chloride, polyvinyl alcohol.

5.4 Miscellaneous fibres: Carbon fibre, glass fibre, boron fibre, ceramic fibre-alumina fibre.

5.5 Brief outline of manufacture of textiles: Fibres to yarn, yarns to fabrics-weaving, knitting, braiding, compound fabric constructions, finishing processes, dyeing and printing.

Unit 6: Rubber Manufacturing and Latex Technology (9 Hrs)

6.1 Natural rubber latex: Composition of latex, conservation, gelation, stability of latex & flocking, chemical modifications of natural latex- prevulcanisation, grafting, halogenations, hydro halogenations.

6.2 Synthetic latex: SBR lattices and its types like XSBR, properties, NBR lattices and its properties, poly chloroprene and its properties, butyl lattices, comparative study of natural, SBR, NBR & poly chloroprene.

6.3 Latex testing: Sampling, total solids, dry rubber content, pH, VFA number, KOH number, mechanical & chemical stability.

6.4 Manufacturing techniques: Dipping-principle & process, foam making-principle, dunlop process, talalay process.

6.5 Physical testing of rubber: Tests on raw materials, tests on rubber compounds, tests on vulcanised samples, tests on products.

6.6 Rubber product manufacturing machinery: Mixing mills, calender machine, extruder, handfly screw press, hydraulic press.

Unit 7: Research Methodology of Chemistry (9 Hrs)

7.1 Purpose of research, conceptualization, elements of a research proposal, research project.

7.2 Types of research: Fundamental, applied and experimental research.

7.3 Chemical literature: Primary, secondary and tertiary sources of literature, literature databases-ScienceDirect, SciFinder, Chemical Abstract.

7.4 Scientific writing: Scientific document, writing of research paper, short communications, review articles, monographs, authored books, edited books and dissertation.

7.5 Important scientific and chemistry journals of various publishers and their impact factors.

7.6 Introduction to: subject index, substance index, author index, h-index.

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CH 88 04 03 ADVANCED ORGANIC CHEMISTRY

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

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

1.1 Survey of organic reactions with special reference to oxidation and reduction. Metal based and non-metal based oxidations of (a) alcohols to carbonyls-chromium (John's oxidation, Collin's oxidation, Sarrett oxidation), manganese, aluminium and DMSO (Swernoxidation, Moffatt–Pfitzner oxidation, Kornblum oxidation, Corey-Kim oxidation) 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 based, ozonolysis) (e) alkenes to alcohols/carbonyls without bond cleavage-hydroboration-oxidation, Wacker oxidation, selenium 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) enzymatic reduction using Baker's yeast.

Unit 2: Modern Synthetic Methods (18 Hrs)

2.1 Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction, Brook rearrangement, Tebbe olefination. Metal mediated C-C and C-X coupling reactions-Heck, Stille, Suzuki-Miyaura, Negishi, Sonogashira, Nozaki-Hiyama-Kishi, Buchwald-Hartwig, Ullmann and Glaser coupling reactions. Click reactions (Huisgen 1,3-dipolar addition).

2.2 Multicomponent reactions: Ugi reaction, Passerini reaction, Biginelli reaction.

Unit 3: Synthetic Reagents (9 Hrs)

3.1 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 trialkyl stannane, aluminum isopropoxide (oxidation and reduction). Reagents such as NBS, DDQ and DCC, Gilmann reagent, DMAP-Borane, PCC, DEAD (Mitsunobu reaction).

Unit 4: Construction of Carbocyclic and Heterocyclic Ring Systems (9 Hrs)

4.1 Synthesis of 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, cation-olefin cyclization, radical-olefin cyclization.

4.2 Inter conversion of ring systems(contraction and expansion): Demjenov reaction, Reformatsky reaction, construction of macrocyclic rings-ring closing metathesis (Grubb's catalyst).

4.3 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 5: Protecting Group Chemistry (9 Hrs)

5.1 Protection and deprotection of hydroxy, carboxyl, carbonyl, and amino groups. Chemo and regio selective protection and deprotection.

5.2 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).

Unit 6: Retrosynthetic Analysis (9 Hrs)

6.1 Basic principles and terminology of retrosynthesis, synthesis of aromatic compounds, one group and two group C-X disconnections, one group C-C and two group C-C disconnections.

6.2 Amine and alkene synthesis: Important strategies of retrosynthesis, functional group transposition, important functional group interconversions, retrosynthesis of D-luciferin, functional equivalents and reactivity-Umpolung reaction (Ireland-Claisen rearrangement).

Unit 7: Supramolecular Chemistry (9 Hrs)

7.1 Concept of molecular recognition, host-guest complex formation, forces involved in molecular recognition.

7.2 Controlling supramolecular topology-the art of building supramolecules.

7.3 Molecular receptors: Cyclodextrins, crown ethers, cryptands, spherands, tweezers, carcerands, cyclophanes, calixarenes, carbon nanocapsules. Dendrimers-molecular trees, rotaxanes-threading molecular rings.

7.4 Applications of supramolecular complexes in perfumery and medicine.

Unit 8: Green Chemistry (9 Hrs)

8.1 Principles of Green Chemistry: Basic concepts, atom economy, twelve principles of green chemistry, principles of green organic synthesis.

8.2 Green alternatives to organic synthesis: Coenzyme catalysed reactions, thiamine catalysed benzoin condensation, green alternatives of molecular rearrangements-pinacol-pinacolone and benzidine rearrangements, electrophilic aromatic substitution reactions, oxidation-reduction reactions, clay catalysed synthesis, condensation reactions, green photochemical reactions.

8.3 Green Solvents: Ionic liquids, supercritical CO_2, fluorous chemistry.

8.4 General principles of microwave and ultrasound assisted organic synthesis.

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GROUP B

ELECTIVE COURSES

CH 89 04 01 MEDICINAL CHEMISTRY

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

Unit 1: Drugs Acting on ANS (18 Hrs)

1.1 Adrenergic stimulants: Phenyl ethanolamine derivatives-adrenaline, isoprenaline, salbutamol, ephedrine, and phenylephrine. Imidazole derivatives-naphazoline, xylometazoline and oxymetazoline.

1.2 Adrenergic blockers: α and β adrenoreceptor antagonists-ergot akaloids, phenoxybenzamine, phentolamine, tolazoline, DCI, propranolol, atenolol, labetolol. Neurone blockers–Bretilium and Xylocholine.

1.3 Cholinergic stimulants: nicotinic and muscarinic receptors, acetyl choline and analogues, pilocarpine, bethanechol and carbachol.

1.4 Cholinergic blockers: tertiary and quaternary antimuscarinics, antispasmodic drugs-dicyclomine, glycopyrrolate, antiulcer drugs-pirenzepine, cycloplegic drugs-tropicamide, homatropine

1.5 Anticholinesterases: Competitive inhibitors-physostigmine and neostigmine.

1.6 Non-competitive inhibitors: organophosphorus compounds, Nerve gases, Cholinesterase regenerators-2 PAM.

1.7 Ganglion blocking agents: mecamylamine and trimethophan

1.8 Curareform drugs: curare alkaloids, erythrina alkaloids and gallamine.

1.9 Synthesis of the following drugs: salbutamol, naphazoline, tolazoline, propranolol, bretilium, carbachol, mecamylamine and gallamine.

Unit 2: Drugs acting on CVS (9 Hrs)

2.1 Cardiotonic drugs: cardiac glycosides-their chemistry and stereochemistry, Digoxin and digitoxin.

2.2 Antiarrhythmic drugs: quinidine, disopyramide, lidocaine, phenytoin and procainamide, β-blockers-propranolol. Calcium channel blockers-verapamil and Neurone blockers-bretilium.

2.3 Antihypertensive Drugs: peripheral antiadrenergics-prazosin and terazosin. Centrally acting drugs-reserpine, clonidine and methyl dopa. β-blockers- propranolol, atenolol

and labetalol. Calcium channel blockers-nifedipine and amlodipine. ACE inhibitors-captopri. Angiotensin receptor blockers-losartan. Diuretics-thiazide diuretics.

2.4 Antianginal drugs: vasodilators-nitrites and nitrates, β-blockers-propranolol. Calcium channel blockers-verapamil and nifedipine. Miscellaneous-dipyridamol and aspirin.

2.5 Anticoagulants: heparin, coumarin derivatives and indane dione derivatives.

2.6 Antilipidemic agents: atherosclerosis (mention only), Statins-lovastatin, simvastatin, fluvastatin, Fibrates-clofibrate, Miscellaneous-bile acid sequestrants and cholestyramine resin.

2.7 Synthesis of the following drugs: procainamide, disopyramide, amlodipine, verapamil, captopril and fluvastatin.

Unit 3: Chemotherapy (27 Hrs)

3.1 Antibiotics: β-lactam antibiotics-penicillins and cephalosporins, natural, biosynthetic and semisynthetic penicillins, tetracyclines and chloramphenicol, a brief study of macrolide antibiotics, aminoglycoside antibiotics, polyene antibiotics, fluoroquinolones.

3.2 Sulphonamides: sulphanilamide, N-substituted sulphanilamide derivatives, mechanism of action, sulphones-dapsone, dihydrofolate reductase inhibitors-trimethoprim and cotrimoxazole.

3.3 Antitubercular agents: first line drugs-isoniazid, rifampicin, pyrazinamide, ethambutol, and streptomycin. Second line drugs-ethionamide, paraaminosalicylic acid and fluoroquinolones.

3.4 Antifungal agents: Antibiotics-amphotericinB, griseofulvin and nystatin. Azole derivatives-ketoconozole,terconozole,fluconozole and clotrimazole. Pyrimidine derivatives- 5 Flucytosine.

3.5 Antiviral drugs: amantidine, interferon and ribavirin. Anti HIV agents- zidovudine, and abacavir. Anti herpes simplex agents-brivudine, vidarabin and acyclovir. Anti-influeza agents-oseltamivir(tamiflu).

3.6 Antiprotozoal agents: Amoebicides-metranidazole and tinidazole. Antimalarials-chloroquine, primaquine, mefloquine, quinacrine and proguanil. Anthelmintics-piperazines and benzimidazoles. Miscellaneous-eflornithine and pentamidine. Synthesis of the following drugs: ampicillin, cephalexin, chloramphenicol, sulphamethoxazole, dapsone, trimethoprim, ethambutol, griseofulvin, clotrimazole, acyclovir, metranidazole, primaquine, mebendazole.

Unit 4: Antineoplastic Drugs **(9 Hrs)**

4.1 Neoplasm-cause therapeutic approaches. Alkylating agents-nitrogen mustards, nitrosourea, aziridines and aryl sulphonates. Antimetabolites-folic acid. Antagonists-purine and pyrimidine antagonists. Antibiotics-anthracyclines, actinomycinD, bleomycin. Plant products-vinca alkaloids, taxol derivatives. Hormones and their antagonists-tamoxifen. Miscellaneos-procarbazine, cisplatin.

4.2 Synthesis of the following drugs: chlorambucil, carmustin, thiotepa, methotrexate, 5-fluoro uracil, procarbazine.

Unit 5: Psychopharmocological Agents **(9 Hrs)**

5.1 Tranquilisers: rauwolfia alkaloids, meprobamate, oxazepim, benzodiazepines, chlordiazepoxide, phenothiazene derivatives.

5.2 Antidepressants: MAO inhibitors-Isocarboxazide, tranylcypromine and phenelzine. Tricyclic compounds-imipramine, trimipramine, amitriptynine, doxepine, amoxapine. Miscellaneous compounds-fluoxetine and trazodone.

5.3 Antipsychotics: phenothiazine and thiothixene derivatives, butyrophenones-haloperidol, droperidon, rauwolfia alkaloids.

5.4 Hallucinogens: triptaminederivatives-DMT, psilocybin, phenylalkylamines-mescaline, lysergic acid derivatives-LSD.

5.5 Synthesis of the following drugs: chlordiazepoxide, meprobamate, imipramine chlorpromazine, tranylcypromine and haloperidol.

Unit 6: Miscellaneous class of compounds **(18 Hrs)**

6.1 Diuretics: common diuretics and their mechanism of action-mercurial and nonmercurial diuretics, carbonic anhydrase inhibitors- acetazolamide and methazolamide, thiazide derivatives-hydrochlorothiazide, Loop diuretics- furosemide and ethacrynic acid, potassium sparing diuretics-amiloride, spironolactone.

6.2 Antihistaminic drugs: histamine and its biological role, H1 antagonists- aminoalkyl ethers, diphenhydramine and doxylamine, ethylenediamine derivatives-pyrilamine, phenothiazines-promethazine, trimeprazine, piperazine derivatives-cyclizines, miscellaneous compounds-cetrizine and cyproheptadine.

6.3 Hypogycemic agents: type 1 and type 2 diabetes, insulin, suphonyl ureas-tolbutamide, acetohexamide and glibenclamide, biguanides-metformin, thiazolidinediones-rosiglitazone.

6.4 Local anaesthetics: clinical application of local anaesthesia, coca and cocaine, hexylcaine, paraaminobenzoic acid derivative-benzocaine, procaine, tetracaine, chloroprocaine, anilides, lidocaine, etiodacaine and prilocaine.

6.5 Antitussives: centrally acting antitussives-opium alkaloids and synthetic substitutes-codaine, noscapine, pholcodine, ethylmorphine, dextromethorphan, Non narcotic antitussives-diphenhydramine, expectorants-terpin hydrate, guaicol and bromhexine.

6.6 Gastrointestinal drugs: purgatives-irritant, osmotic, bulk and lubricant purgatives, Antacids-systemic and non systemic antacids, H2 antagonists-cimetidine and ranitidine, proton pump inhibitors-omeprazole and pantaprazole, digestants, carminatives and antidiarrheals.

6.7 Synthesis of the following drugs: acetazolamide, chlorthiazide furosemide, ethacrynic acid, amiloride, diphenhydramine, pyrilamine, promethazine, omeprazole, tolbutamide, phenformin, benzocaine, procaine lidocaine, dextromethorphan.

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CH 89 04 02 ADVANCES IN POLYMER SCIENCE AND TECHNOLOGY

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

Unit 1: Specialty Polymers (18 Hrs)

1.1 Poly electrolytes-water soluble charged polymers, ionomers (ion containing polymers), conducting polymers, solid polymer electrolytes (SPE), electroluminescent polymers, fluoropolymers, block copolymers(multiphase polymers), polymer colloids, thermoplastic elastomers(TPE), polyblends (heterogeneous plastics), inter penetrating network (IPN) polymers, thermally stable polymers, telechelic polymers (functional polymers) polymer microgel, biomedical polymers.

1.2 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, application of liquid crystalline polymers.

1.3 Dendritic polymers: Origin of dendrimers, structure, properties, design and synthesis-divergent growth method, convergent growth method, medicinal application.

1.4 Introduction to: Polymers for organic light-emitting diodes (OLEDs), organic and hybrid solar cell, supramolecular polymer science.

Unit 2: Adhesives and Surface Coating (9 Hrs)

2.1 Adhesives: Introduction, theory, surface treatment, joint design, physical nature of adhesives, types of adhesives, natural glues, applications, elastomer adhesives, synthetic adhesives, olefinic polymer adhesives, types of epoxy adhesives, inorganic adhesives, bio adhesives, test methods in determining the strength and properties of adhesives.

2.2 Surface coating: Introduction, types of coating, drying oils, types of resins, surfactants, surface preparation, coating methods, solvent selection, methods of coating, theory of powder coating, application of powder coating, curving process. Corrosion, electroplating, hazards and safety measures in paint industry.

Unit 3: Polymer Blends and Composites (18 Hrs)

3.1 Polymer blends: Classification, principles and methods involved in the preparation of different polymer blends, study of polymer blends and alloys on the basis of miscibility, criteria for selection of polymer. Compatibility of blends-principles of solubility and compatibility, thermodynamics of miscibility, mechanical compatibility. Phase morphology-Phase separation behaviour, morphology of blends and its determination- electron microscopy- domain structure.

3.2 Introduction to rheology of polymer blends: Relevance in processing, rheology–phase morphology relationships and their relevance, micro rheology, rheological models-solution, and suspension models.

3.3 Industrial applications of polymer blends.

3.4 Polymer composites: Fundamental concepts, factors influencing the performance of polymer composites-aspect ratio, void content, length of the fibre, nature of the fibre. Structure property relationship between fibre and matrix, modifications of the fibre surface, degree of interaction between fibre and matrix, wetting behaviour, degree of cross linking etc.,

3.5 Processing of thermoplastic composites: Types of processing methods, solution, film, lamination, sandwitch etc., processing conditions, advantages and disadvantages.

3.6 Fabrications of thermoset composites: Hand layup method, compression and transfer moulding, pressure and vacuum bag process, filament winding, protrusion, reinforced RIM, RRIM, injection moulding of thermosets, SMC and DMC.

3.7 Nano-composites: Definition, types, methods of fabrication, characterization. Polymer/CNTs and Polymer/Nanoclay based composites, properties and their functional applications.

Unit 4: Polymer Compounding and Processing (18 Hrs)

4.1 Polymer mixing: Introduction, basic concepts, mechanism of mixing and dispersion, mixing of solid-solid, liquid-liquid and liquid-solid, dispersive mixing, distributive mixing and laminar mixing, mixing indices, kinetics of mixing, rheology of filled polymers.

4.2 Compounding: Introduction, types and characteristics of compounds-polymer blends, polymer formulations, filled polymers and polymer composites, compounding practice, mixing types, solid additives, morphology of filler additives, compatibilizers-mechanism and theory, filler surface modification and interfacial agents, dispersion of polymer nanoparticles in polymer melt, fillers and reinforcements *viz.* carbon black, ZnO, calcium carbonate, titanium oxide, nano clay, glass fibers, organic fillers, nanofillers. Compounding ingredients for rubber-fillers, reinforcing, semi reinforcing and nonreinforcing, 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.

4.3 Polymer processing: Casting-die casting, rotational casting, film casting, thermoforming, foaming, lamination, reinforcing, processing of fibres-dry spinning, wet spinning, melt spinning, moulding processes-compression moulding, injection moulding, transfer moulding, blow moulding, extrusion moulding, calendaring.

Unit 5: Fibre Science and Technology (9 Hrs)

5.1 Basic concepts, structural attributes of fibres, fibre characteristics.

5.2 Natural fibres: Natural fibres of vegetable origin, the seed and fruit fibres, natural fibres of animal origin-silk, natural mineral fibre.

5.3 Man-made fibres: Introduction, spinning, semi-synthetic fibres from cellulose, regenerated protein fibres, synthetic fibres-rayon, polyethylene terephthalate, nylon 6 and nylon 66, polyolefins, polyvinyl chloride, polyvinyl alcohol.

5.4 Miscellaneous fibres: Carbon fibre, glass fibre, boron fibre, ceramic fibre-alumina fibre.

5.5 Brief outline of manufacture of textiles: Fibres to yarn, yarns to fabrics-weaving, knitting, braiding, compound fabric constructions, finishing processes, dyeing and printing.

Unit 6: Rubber Manufacturing and Latex Technology (9 Hrs)

6.1 Natural rubber latex: Composition of latex, conservation, gelation, stability of latex & flocking, chemical modifications of natural latex- prevulcanisation, grafting, halogenations, hydro halogenations.

6.2 Synthetic latex: SBR lattices and its types like XSBR, properties, NBR lattices and its properties, poly chloroprene and its properties, butyl lattices, comparative study of natural, SBR, NBR & poly chloroprene.

6.3 Latex testing: Sampling, total solids, dry rubber content, pH, VFA number, KOH number, mechanical & chemical stability.

6.4 Manufacturing techniques: Dipping-principle & process, foam making-principle, dunlop process, talalay process.

6.5 Physical testing of rubber: Tests on raw materials, tests on rubber compounds, tests on vulcanised samples, tests on products.

6.6 Rubber product manufacturing machinery: Mixing mills, calender machine, extruder, handfly screw press, hydraulic press.

Unit 7: Research Methodology of Chemistry (9 Hrs)

7.1 Purpose of research, conceptualization, elements of a research proposal, research project.

7.2 Types of research: Fundamental, applied and experimental research.

7.3 Chemical literature: Primary, secondary and tertiary sources of literature, literature databases-ScienceDirect, SciFinder, Chemical Abstract.

7.4 Scientific writing: Scientific document, writing of research paper, short communications, review articles, monographs, authored books, edited books and dissertation.

7.5 Important scientific and chemistry journals of various publishers and their impact factors.

7.6 Introduction to: subject index, substance index, author index, h-index.

References

1. P. Bahadur, N. V. Sastry, Principles of Polymer Science, Narosa publishing house Pvt. Ltd., New Delhi, 2005.
2. M.S. Bhatnagar, A Textbook of Polymers, Vol II, S. Chand & Company Ltd., 2004.
3. Premamoy Ghosh, Fibre Science & Technology, McGraw-Hill professional, 2004.
4. D.C. Blackley, Polymer lattices: Science and Technology, Springer Netherlands, 2012.
5. J. M. Martin, W. K. Smith, Hand Book of Rubber Technology, CBS Publishers, 2004.
6. Joel R. Fried, Polymer Science and Technology, 3rd Edn., 2014.
7. Zehev Tadmor, Costas G. Gogos, Principles of Polymer Processing, 2nd Edn., 2006.
8. Jean M. J. Fréchet, Donald A. Tomalia, Dendrimers and other Dendritic Polymers, Wiley, 2002.
9. Muralisrinivasan, Natamai, Subramanian, Polymer Blends and Composites: Chemistry and Technology, Scrivener Publishing LLC, 2017.
10. Lloyd M. Robeson, Polymer Blends, Hanser Gardner Publications, U.S.A, 2007.
11. Leszek A. Utracki, Polymer Alloys and Blends: Thermodynamics and Rheology, Hanser Gardner Publications, 1989.
12. Paul D Leedy, Jeanne E. Ormrod and Jeanne Ellis Ormrod, Practical Research: Planning and Design, Prentice Hall, 2004.
13. John W. Creswell, Qualitative Research & Evaluation Methods, 2008.
14. Ezio Martuscelli, Polymer Blends: Processing, Morphology, and Properties, Springer-Verlag New York Inc., 2011.
15. P. M. Ajayan, L.S. Schadler, P. V. Braun, Nanocomposites - Science and Technology, Wiley-VCH, 2004.
16. P. M. Ajayan, L.S. Schadler, P. V. Braun, Nanocomposites - Science and Technology, Wiley-VCH, 2004.

CH 89 04 03 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 absorptionspectrometry. 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 (1H, 13C, 32P). 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

1. J. M. Mermet, M. Otto, R. Kellner, Analytical Chemistry, Wiley-VCH, 2004.
2. D. A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College Pub., 2007.
3. R. D. Brownn, Introduction to Instrumental Analysis, McGraw-Hill, 1958.
4. H.H. Willard, L.L. Merritt, J. A. Dean, Instrumental Methods of Analysis, Van Nostrand, 1974.
5. G. D. Christian, J.E. O'Reilly, Instrumental Analysis, Allyn & Bacon, 1986.
6. J. H. Kennedy, Analytical Chemistry: Principles, Saunders College Pub., 1990.
7. J. G. Dick, Analytical Chemistry, R.E. Krieger Pub., 1978.
8. E. D. Howe, Fundamentals of Water Desalination, Marcel Dekker, 1974.
9. H. G. Heitmann, Saline Water Processing, VCH

SEMESTERS 3 AND 4

CH 05 04 05 POLYMER PREPARATIVE PRACTICAL-2

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

PART I: Preparation of Polymers

Any six preparations of the following may be carried out:

1. Preparation of nylon -6,6 (Interfacial polycondensation)
2. Preparation of PMMA (free radical bulk polymerization)
3. Preparation of polyacrylamide (free radical polymerization)
4. Preparation of polyacrylamide (redox polymerization)
5. Preparation of glyptal resin
6. Preparation of linear polystyrene (free radical polymerization)
7. Preparation of crosslinked polystyrene (suspension polymerization)
8. Preparation of phenol formaldehyde resin (resoles and novolacs)
9. Preparation of urea formaldehyde resin
10. Preparation of polyaniline
11. Preparation of aniline formaldehyde resin

PART II: Latex Analysis

1. Determination of total solid content of latex
2. Determination of alkalinity of latex
3. Determination of dry rubber content of latex
4. Determination of volatile fatty acid number of latex
5. Determination of viscosity of latex
6. Determination of KOH number

References

1. E.A. Collins, J. Bares, F.W. Billmeyer, Experiments in Polymer Science, Wiley-Interscience, 1973.
2. S.H. Pinner, A Practical Course in Polymer Chemistry, Pergamon, 1961.
3. D. Braun, H. Cherdron, W. Kern, Practical Macromolecular Organic Chemistry,3rd Edn, Harwood Academic Pub., 1984.
4. S.R. Sandler, W. Karo, Polymer Synthesis, Vol.1, Academic Press, 1992.

5. S.R. Sandler, W. Karo, Polymer Synthesis, Vol.2, Academic Press, 1993.
6. S.R. Sandler, W. Karo, Polymer Synthesis, Vol.3, Academic Press, 1998.
7. D. C. Blackley, Polymer Latices, Vol.1, 2 & 3, 2nd Edn., Springer, 1997.
8. W.C. Wake, Analysis of Rubbers and Rubber like Polymers, 2nd Edn, Wiley-Interscience, 1969.

CH 05 04 06 POLYMER CHARACTERIZATION PRACTICAL-2

Credit: 3 **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 Tg, Tm 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.

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

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

CH 05 04 07 POLYMER PROCESSING AND TESTING PRACTICAL-2

Credit: 3 **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

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

MODEL QUESTION PAPERS

QP Code **Reg. No. …..**

Name ……

M.Sc. Degree (C.S.S) Examination

First Semester

Faculty of Science-Polymer Chemistry

CH 50 01 01- Organometallics and Nuclear Chemistry

(Common for all branches of Chemistry)

(2019 admissions onwards)

Time: Three hours Max. Weight: 30

Section- A

(Answer any **eight** questions. Each question carries a weight of 1)

1. What is synergism?
2. Define the term "isolobal".
3. Give an example for a β-elimination reaction.
4. What are Ziegler- Natta catalysts?
5. What is Bohr effect?
6. What is *cis*-platin? What are its important applications?
7. What is radiation polymerisation?
8. How is nuclear reaction cross section related to reaction rate?
9. List the important functions of biological membranes.
10. Give an example for the use of palladium catalysts in the formation of C-N bond.

(8 x 1 = 8)

Section B

(Answer any **six** questions. Each question carries a weight of 2)

11. Discuss the bonding in ferrocene.
12. What are oxidative addition reactions? Discuss the important mechanisms involved in oxidative additions.
13. What is Wilkinson's catalyst? What are its uses? Describe alkene hydrogenation using Wilkinson's catalyst with the help of Tolman catalytic loops.
14. Explain the structure and functions of carbonic anhydrase, carboxypeptidase A and superoxide dismutase.

15. Write a note on the synthesis of transuranic elements.
16. Outline the role of chlorophyll in photosynthesis.
17. What are insertion reactions? Discuss insertion of alkenes and alkynes in the Ar-H bond.
18. Write a note on carbonyl clusters.

(**6 x 2 = 12**)

Section C

(Answer any **two** questions. Each question carries a weight of 5.)

19. What are π-bonding ligands? Explain the preparation, properties, structure and bonding of simple mono and binuclear metal carbonyls, metal nitrosyls, metal cyanides and dinitrogen complexes.
20. a) Write a note on carbonylation reactions.

    b) Write a note on asymmetric catalysis. Discuss asymmetric hydrogenation, isomerisation and epoxidation.
21. Discuss oxygen transport mechanism. What are the functions of haemoglobin and myoglobin in oxygen transport?
22. a) Discuss important analytical applications of radioisotopes.

    b) Outline fluxional isomerism of allyl, cyclopentadienyl and allene systems.

(**2 x 5 = 10)**

QP Code: **Reg. No. …..**

Name ……

M Sc Degree (C.S.S) Examination

First Semester

Faculty of Science-Chemistry

CH 50 01 02 STRUCTURAL AND MOLECULAR ORGANIC CHEMISTRY

(Common for all branches of Chemistry)

(2019 admissions onwards)

Time: Three hours Max. Weight: 30

Section- A

(Answer any **eight** questions. Each question carries a weight of 1)

1. Explain inductive effect with suitable examples
2. What is meant by 1)chirality 2)diastereoisomers
3. What is meant by topicity? Explain by examples
4. Explain the mechanism of photo Fries rearrangement
5. Give the mathematical form of Hammet equation and explain the terms.
6. What is primary kinetic isotope effect?
7. What type of compounds are named by using the prefixes erythro and threo? Give one example.
8. What is Hammond postulate?
9. Draw the structure of the following molecules
    1. (2R, 3S)-2,3-dichloropentane
    2. S-1-bromo-1-chloropropane
10. Draw the conformations of cyclohexane derivatives.

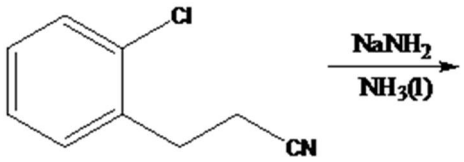
(8 x 1 = 8)

Section B

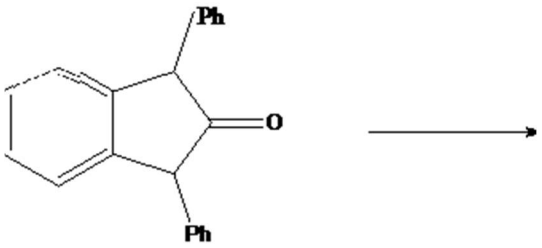
(Answer any **six** questions. Each question carries a weight of 2)

11. Predict the product and explain the mechanism

a)



b)



12. What are the applications of Taft equation in ester hydrolysis?

13. Write a note on Fullerenes and Graphene.

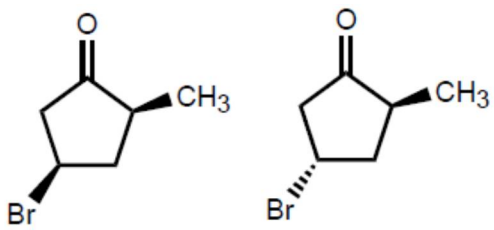
14. What are hard and soft acids? Use HSAB principle to distinguish them

15. Differentiate between kinetic and thermodynamic control of organic reactions.

16. Explain Curtin Hammett principle

17. Explain with example how NMR used to distinguish enantiotopic/ diastereotopic ligands.

18. Is it theoretically possible to separate the pair of compounds below by distillation? Explain briefly.



(6 x 2 = 12)

Section C

(Answer any **two** questions. Each question carries a weight of 5.)

19. a) Illustrate the conformational studies of i) Decalin ii) Adamanatane

    b)Explain the mechanism of semipinacolic deamination.

20. How do mesomeric ,hyperconjugative and steric effects influence the strength of organic bases ?

21. Explain the Nucleophilic substitution reactions in aromatic systems

22. Explain in detail about: a) Carbon based chiral centers. b) N based chiral centers. c) S based chiral centers.

(2 x 5 = 10)

QP Code **Reg. No. …..**

Name ……

M. Sc. Degree (C.S.S) Examination, 2019

First Semester

Faculty of Science-Polymer Chemistry

CH 50 01 03-Quantum Chemistry and Group Theory

(Common for all branches of Chemistry)

(2019 admissions onwards)

Time: Three hours Max. Weight: 30

Section- A

(Answer any **eight** questions. Each question carries a weight of 1)

1. Predict the point group of (i) glyoxal (ii) cis-$[Co(en)_2Cl_2]^+$
2. Explain cyclic groups?
3. What are sub groups? How many sub groups are possible for D_3h?
4. List all the elements of benzene
5. Obtain the inverse of Sn^m, when n is even and m is even/odd
6. What are nodes? How many nodes are there in the plot of radial probability function for a 4p orbital?
7. Given below are the certain wave functions. State which of them are eigen function of d^2/dx^2. If so give the eigen values : a) A+B sin ax; (b) A cos ax (c) Ae^{ax}
8. Define recursion relation
9. What are Ladder operators?
10. Explain the term spherical harmonics.

(8 x 1 = 8)

Section B

(Answer any **six** questions. Each question carries a weight of 2)

11. Show that L^2 and L_y commute
12. Show that the normalized wave function for a particle in a 3D box with sides of length a, b and c is $\Psi(x,y,z) = (8/abc)^{1/2}$ $(sinnx\Pi x/a)$ $(si\square\square ny\Pi y/b)(sinnz\Pi z/c)$

and discuss the degeneracies of the first few energy levels.

13. Explain the postulate of spin by Uhlenbeck and Goudsmith, discovery of spin-Stern Gerlach experiment.
14. Derive an expression for wave equation of particle on a ring
15. Prepare GMT for (i) C_{2h} (ii) C_{3v}
16. Discuss screw axis and glide planes for crystals.
17. Derive the matrix for C_n and hence S_n element.
18. State and explain Great Orthogonality Theorem

(**6 x 2 = 12**)

Section C

(Answer any **two** questions. Each question carries a weight of 5.)

19. Construct the character table for C_3v and hence obtain the SALC.
20. Obtain the matrix representations for symmetry elements of NH_3
21. Explain 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
22. What are hermite polynomials? How they are used for solving Schrödinger equation for a harmonic oscillator.

(**2 x 5 = 10)**

QP Code **Reg. No. …..**

Name ……

M. Sc. Degree (C.S.S) Examination, 2019

First Semester

Faculty of Science-Polymer Chemistry

CH 50 01 04- Thermodynamics, Kinetic theory and Statistical Thermodynamics

(Common for all branches of chemistry)

(2019 admissions onwards)

Time: Three hours Max. Weight: 30

Section- A

(Answer any **eight** questions. Each question carries a weight of 1)

1. Explain the term fugacity. What is the physical significance of fugacity?
2. What are Maxwell relations? Explain.
3. Explain the term chemical potential? Derive the Gibbs-Duhem equation?
4. Define thermodynamic excess functions. Formulate expression for excess Gibbs free energy.
5. Define mean free path and collision frequency. How do they vary with pressure and temperature?
6. Explain the terms (a) phase space,(b)microstates, (c) macrostates
7. Derive the relation between thermodynamic probability and entropy.
8. Briefly explain the statistical formulations of third law of thermodynamics.
9. What is partition function ? How is it factorised into contributing parts ?
10. Distinguish between Bosons and Fermions**.**

(8 x 1 = 8)

Section B

(Answer any **six** questions. Each question carries a weight of 2)

11. What is meant by thermodynamics of mixing? Derive Gibbs-Duhem- Margules equation.
12. Derive Gibb's –Helmholtz equation. What are it's applications.
13. Derive Maxwell's law of distribution of velocities.
14. Explain Bose-Einstein condensation.
15. Derive Sackur – Tetrode equation applicable to monoatomic gases.

16. The free energy change ΔG accompanying a given process is -85.77 kJ at 25^oC and –83.68 kJ at 35^oC. Calculate the change in enthalpy (ΔH) for the process at 30^oC.
17. Calculate the translational entropy of gaseous iodine at 298K and 1 atm.
18. Calculate the rotational partiton function for hydrogen molecule at 300K. Moment of inertia of hydrogen molecule is $4.59x10^{-47}Kgm^2$ symmetry number σ=2.

(**6 x 2 = 12**)

Section C

(Answer any **two** questions. Each question carries a weight of 5)

19. What is Nernst heat theorem? Explain the determination of absolute entropies using third law?
20. Discuss about a three component system taking suitable example and give its graphical representation.
21. (a) Derive an expression for Fermi-Dirac statistics (b) Give comparative account of the three statistics.
22. Derive Debye theory of heat capacity of solids. How does it differ from Einstein theory?

(2 x 5 = 10)

QP Code **Reg. No. …..**

Name ……

M. Sc. Degree (C.S.S) Examination, 2019

Second Semester

Faculty of Science-Polymer Chemistry

CH 50 02 01 - Coordination Chemistry

(2019 admissions onwards)

Time: Three hours Max. Weight: 30

Section- A

(Answer any **eight** questions. Each question carries a weight of 1)

1. What is chelate effect?
2. What is nephelauxetic effect?
3. Write the term symbol for a d1 configuration.
4. What are the demerits of Orgel diagrams?
5. Give an example for mixed outer and inner sphere reactions.
6. What do you mean by hard and soft ligands?
7. How do 4f orbitals differ from 5f orbitals?
8. Give two applications of organolanthanoid complexes in catalysis.
9. Give an example for the use of coordination compounds as catalysts in asymmetric synthesis.
10. Discuss effect of H+ on the rates of substitution of chelate complexes.

(8 x 1 = 8)

Section B

(Answer any **six** questions. Each question carries a weight of 2)

11. Write a note on the thermodynamic aspects of complex formation.
12. Discuss Jahn Teller effect.
13. Explain trans-effect theory for the substitution reactions in square planar complexes.
14. Sketch the Tanabe-Sugano diagram for [V(H2O)6]3+.
15. a) Discuss geometrical isomerism in octahedral complexes.
    b) Write a note on electronic and steric factors affecting linkage isomerism.
16. Compare the coordination chemistry of lanthanoids and actinoids with special reference to electronic spectra and magnetic properties.

17. Discuss inner sphere and outer sphere mechanisms of electron transfer reactions.
18. Give an account of qualitative treatment for the correlation diagram of d9 system.

(6 x 2 = 12

Section C

(Answer any **two** questions. Each question carries a weight of 5)

19. Give an account of crystal field theory. Discuss splitting of d orbitals in octahedral, tetrahedral, square planar, square pyramidal and triagonal bipyramidal fields. List the drawbacks of crystal field theory.
20. Give an account of magnetic properties of complexes.
21. Write a note on optical isomerism in octahedral complexes. Describe resolution of optically active complexes and determination of absolute configuration of complexes by ORD and circular dichroism.
22. Give an account of kinetics and mechanism of substitution in octahedral complexes with special reference to dissociative and associative mechanisms, base hydrolysis and solvolytic reactions.

(2 x 5 = 10)

QP Code **Reg. No. …..**

Name ……

M. Sc. Degree (C.S.S) Examination, 2019

Second Semester

Faculty of Science-Polymer Chemistry

CH 50 0202- Organic Reaction Mechanism
(Common for all branches of Chemistry)

(2019 admissions onwards)

Time: Three hours Max. Weight: 30

Section- A

(Answer any **eight** questions. Each question carries a weight of 1)

1. Give one example each for the insertion reaction and addition reaction of carbenes.
2. Distinguish between classical and non-classical carbocations
3. Briefly explain the Woodward Hoffmann rule
4. Write a note on oxymercuration
5. How can you obtain cycloheptanone from cyclohexanone
6. Discuss the regioselectivity of addition reactions with suitable examples.
7. What is Clemmenson reduction. Give mechanism
8. Write down the product and mechanism of the following reaction
9. Discuss Baldwin's rules.
10. What are Grignard reagents? Write down their applications?

(8 x 1 = 8)

Section B

(Answer any **six** questions. Each question carries a weight of 2)

11. Discuss anti Markovnikov's addition mechanism
12. Identify the reaction and discuss the mechanism of the following reaction
13. Write a note on Mannich reaction
14. Use appropriate reagents and discuss the mechanism of the reaction
15. Give the mechanism and stereochemistry of Diels- Alder reaction
16. Write briefly on Lossen rearrangement
17. What are enolates. Compare them with enamines in synthetic applications
18. Discuss the mechanism of Stobbe condensation and its synthetic applications

(6 x 2 = 12)

Section C

(Answer any **two** questions. Each question carries a weight of 5)

19. What are carbanions? Discuss their formation, structure and stability. What are their importance as reaction intermediates?
20. Give the mechanism of the following reactions.

    1) Wolf rearrangement 2) Michael addition 3) Cannizaro reaction 4) Darzen condensation
21. What are the different types of pericyclic reactions? Discuss the importance of pericyclic reactions in organic synthesis.
22. i) How can you generate nitrenes?

    ii) Differentiate between SN1 and SN2 reactions.

    iii) Discuss the mechanism of halolactonisation.

(2 x 5 = 10)

QP Code **Reg. No. …..**

Name ……

M. Sc. Degree (C.S.S) Examination, 2019

Second Semester

Faculty of Science-Polymer Chemistry

CH 50 02 03-Chemical Bonding and Computational Chemistry
(Common for all branches of Chemistry)

(2019 admissions onwards)

Time: Three hours Max. Weight: 30

Section- A

(Answer any **eight** questions. Each question carries a weight of 1)

1. What are slater determinants?
2. State and Explain Variation theorem
3. State and explain Non crossing rule in quantum mechanics
4. Explain Hellmann-Feynmann theorem.
5. Find out the characters for all the symmetry operations of NH_3 molecule using Cartesian coordinates.
6. What are the group theoretical selection rules for an electronic transition to be allowed?
7. Explain AMBER.
8. What is CHARMM? Explain its use in molecular mechanics.
9. What is Koopman's Theorem?
10. Write a short note on Independent Electron Approximation

(8 x 1 = 8)

Section B

(Answer any **six** questions. Each question carries a weight of 2)

11. Illustrate variation theorem using the trial wave function x(a-x) for particle in a one dimensional box
12. Explain Huckelmolecular orbital theory of Butadiene and Benzene
13. Explain how group theory helps to predict optical activity
14. Using Direct Product Tables, predict the electronic transitions of C_2v and C_3v molecules.
15. What are the important assumptions used in HFSCF method ?
16. Explain how to build a Z-matrix?
17. Compare MOT and VBT

18. Explain the Kohn-Sham approach used in DFT?

(6 x 2 = 12)

Section C

(Answer any **two** questions. Each question carries a weight of 5)

19. How GAMESS is input file prepared? Illustrate with reference to water molecule?

20. Using group theory, derive the allowed electronic transitions in formaldehyde.

21. Explain Perturbation Method? Illustrate with Helium as Example

22. Explain molecular orbital theory and derive an expression for energy and wave function of Hydrogen molecule.

(2 x 5 =10)

QP Code **Reg. No. …..**

Name ……

M. Sc. Degree (C.S.S) Examination, 2019

Second Semester

Faculty of Science-Polymer Chemistry

CH 50 02 04–Molecular Spectroscopy
(Common for all branches of Chemistry)

(2019 admissions onwards)

Time: Three Hours Maximum Weight: 30

Section A

(Answer any **eight** questions. Each question carries a weight of 1)

1. What is FID and FT in NMR spectroscopy?
2. What is Born Oppenheimer approximation? Explain the cases where the Born Oppenheimer approximation breaks down.
3. What is fermi resonance? Give one example.
4. Explain mutual exclusion principle.
5. Which of the following molecules exhibit pure rotational spectra? HF, NH_3 ,H_2O , CO, CH_4 , BF_3 , CO_2 , F_2 .
6. Differentiate between first order and second order NMR spectra
7. What are fine structure and hyperfine structure in ESR spectrum?
8. What is Resonance Raman Spectrum?
9. What is finger print region in IR?
10. Discuss Frank condon principle.

(8 × 1 =8)

Section B

(Answer any **six** questions. Each question carries a weight of 2

11. Explain the basic principle of NQR spectroscopy.
12. Give the applications of ESR and Mossbauer methods in spectroscopy
13. Explain the terms chemical shift, coupling constant and factors influencing coupling constant in NMR spectroscopy
14. The first line in the rotational spectrum of NO appears at 1.72 cm^{-1} and its force constant is 1608 Nm^{-1}. Calculate the internuclear distance in A^0, vibrational frequency in cm^{-1} and energy in joules required for J = 3 to 4 rotational transition.

15. The first three vibrational energy of HCl were found to be at 2886, 5668 and 10923 cm^{-1}. Calculate the anharmonicity constant, zero point energy and the equilibrium oscillation frequency. Calculate the centrifugal distoration constant if the rotational constant is 21.18 cm^{-1} .
16. Discuss photoelectron spectroscopy.
17. Explain the various relaxation methods in NMR..
18. What is meant by normal mode of vibration? How many normal modes of vibration do the following molecules have? NH_3 , HCN , SO_2

(6 × 2 = 12)

Section C

Answer any two questions. Each question carries a weight of 5

19. Explain the following in NMR spectroscopy
    a) Larmor Precision
    b) Chemical shift and its representation
    c) Magic angle spinning
20. Explain the classical theory of Raman spectroscopy.
21. Discuss the theory and applications of NQR Spectroscopy.
22. Write note on:
    a) Resonance fluorescence
    b) Predissociation
    c) Mechanism of Laser action
    d) Polarized and depolarized Raman lines

(5 × 2 = 10)

QP Code **Reg. No. …..**

Name ……

M. Sc. Degree (C.S.S) Examination, 2019

Third Semester

Faculty of Science-Polymer Chemistry

CH 50 03 01 - Structural Inorganic Chemistry
(Common for Chemistry/Analytical Chemistry/Polymer Chemistry)

(2019 admissions onwards)

Time: Three hours Max. Weight: 30

Section- A

(Answer any **eight** questions. Each question carries a weight of 1)

1. Give an account of wurzite structure.
2. What are Cooper pairs?
3. What are the important applications of poly(ferrocenylsilane)s?
4. How is silica glass prepared?
5. Give an account of the applications of magnetic nanoparticles in MRI.
6. Write a short note on organometallic dendrimers.
7. What are the important medical applications of boron clusters?
8. What are one dimensional conductors?
9. Write a short note on the super conductivity of fullerenes.
10. Give one example each forcatenation and heterocatenation.

(8 x 1 = 8)

Section B

(Answer any **six** questions. Each question carries a weight of 2)

11. Give an account of spinel and inverse spinal structures.
12. Write a note on free electron theory of solids.
13. Outline the magnetic properties of spinels, ilmenites and perovskites.
14. Write a note on heteropoly acids of Mo and W.
15. Discuss the structure and bonding in sulphur-nitrogen compounds.
16. Give an account of the preparation, structure and bonding in cages and clusters of germanium and tin.
17. Write a note on polymers based on ferrocene. List their applications.
18. Explain different methods for the preparation of thin films.

(6 x 2 = 12)

Section C

(Answer any **two** questions. Each question carries a weight of 5)

19. Give an account of phase transitions in solids. Discuss different types of phase transitions and kinetics of phase transitions.
20. Explain band theory of solids. Discuss applications of band theory to transition metal compounds and compounds like NaCl, MgO and fullerenes. Outline the mechanism of intrinsic and extrinsic semiconductors.
21. a) Give an account of the synthesis, structure and applications of silicones and zeolites.

    b) Discuss the preparation, properties and structures of cage like structure of phosphorous and cages of boron with aluminium and indium.
22. Give an account of the applications of magnetic nanoparticles.

    b) What are type I and type II superconductors? Discuss BCS theory of superconductivity.

(2 x 5 = 10)

QP Code **Reg. No. …..**

Name ……

M. Sc. Degree (C.S.S) Examination, 2019

Third Semester

Faculty of Science-Polymer Chemistry

CH 05 03 02- Chemical Kinetics and Surface Chemistry

(2019 admissions onwards)

Time: Three hours Max. Weight: 30

Section- A

(Answer any **eight** questions. Each question carries a weight of 1)

1. Give the significance of $\Delta S^{\neq}$
2. What is Skrabal diagram?
3. Mention important applications of Surface Enhanced Raman Scattering
4. What is zeta potential?
5. What is the principle of microscopic reversibility?
6. What is quantum yield ?
7. Write down the advantages of coulometry?
8. Give an account of the pharmaceutical applications of DTA
9. What are the disadvantages of AES?
10. List the important applications of ESCA.

(8 x 1 = 8)

Section B

(Answer any **six** questions. Each question carries a weight of 2)

11. Write notes on applications of nano materials in catalysis
12. Discuss the kinetics of H_2-Br_2 Reaction
13. Write a note on the use of SEM and TEM in the study of surfaces
14. Derive Michelis-Menten equation.
15. Discuss the principle, instrumentation and applications of TGA
16. Give an account of the principles and applications of FES
17. Write a note on the photochemistry of vision
18. Write a short essay on application of coulometric titrations

(6 x 2 = 12)

Section C

(Answer any **two** questions. Each question carries a weight of 5.)

19. What are the factors determining reaction rates in solutions? Derive Bronsted-Bjerrum equation. Discuss primary and secondary kinetic salt effect
20. Outline Langmuir and BET theories of adsorption. Describe Use of Langmuir and BET isotherms for surface area determination
21. (a) What are coupled reactions? Discuss the role of ATP in bioenergetics b) Give an account of thermodynamic aspects of metabolism and respiration and glycolysis
22. Describe the optical, electrical and magnetic properties of nano materials

(2 x 5 = 10)

QP Code **Reg. No. …..**

Name ……

M. Sc. Degree (C.S.S) Examination, 2019

Third Semester

Faculty of Science-Polymer Chemistry

CH 05 03 03- Concepts of Polymer Chemistry

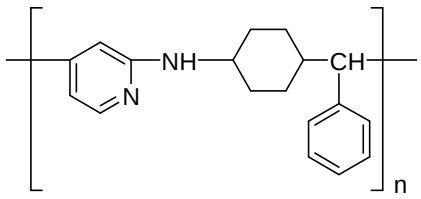
(2019 admissions onwards)

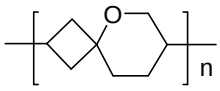
Time: Three hours Max. Weight: 30

Section- A

(Answer any **eight** questions. Each question carries a weight of 1)

1. Name each of the polymers by the IUPAC system

a) 

b) 

2. Give one reaction of poly(vinyl acetate)
3. What do you mean by accelerated sulphur vulcanization?
4. Briefly explain living polymerisation
5. Give an account of molecular forces in polymers
6. What is hydrophobic interaction?
7. What are optically active monomers? Give one example
8. Write the mechanism of copolymerisation
9. What do you mean by tacticity in polymers
10. Discuss the conformations of poly ethylene

(8 x 1 = 8)

Section B

(Answer any **six** questions. Each question carries a weight of 2)

11. Explain esterification and etherification reactions of cellulose
12. Describe radical graft polymerisation using suitable example
13. Write the mechanism of vinyl polymerization
14. Give a short note ring opening polymerization
15. Explain anionic and cationic graft polymerization

16. Discuss stereoisomerism in disubstituted ethylenes
17. Describe stereoregularity in isotactic, syndiotactic, and atactic polypropenes
18. Write notes on radiation crosslinking

(**6 x 2 = 12**)

Section C

(Answer any **two** questions. Each question carries a weight of 5.)

19. Write an essay on polymer supports in solid phase peptide and protein synthesis.
20. Explain the following:

    (a) Polymerisation in supercritical fluids (b) polymerisation in ionic liquids (c) click chemistry for polymerisation (d) Ziegler Natta polymerization
21. Give detailed description of the following living radical polymerization:

    (a) Atom transfer radical polymerization (b) stable free-radical polymerisation (c) radical addition-fragmentation transfer
22. Describe the following polymerisation techniques:

    (a) Bulk polymerization (b) solution polymerization (c) suspension polymerization (d) emulsion polymerization

(**2 x 5 = 10**)

QP Code **Reg. No. …..**

Name ……

M. Sc. Degree (C.S.S) Examination, 2019

Third Semester

Faculty of Science-Polymer Chemistry

CH 50 03 04 – Spectroscopic Methods in Chemistry
(Common for all branches of Chemistry)

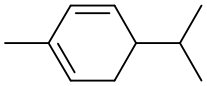
(2019 admissions onwards)

Time: Three hours Max. Weight: 30

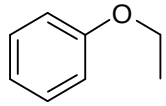
Section- A

(Answer any **eight** questions. Each question carries a weight of 1)

1. Calculate the λ_{max} for the compound



2. Which of the following isomers of pentadiene will show the largest wavelength of UV absorption? Give reason.
   i) CH_2=CH-CH=CH-CH_3 ii) CH_2=CH-CH_2-CH=CH_2
3. 2-Hydroxy-3-nitroacetophenone shows two carbonyl stretching frequencies at 1692 and 1658 cm^{-1}. Explain.
4. C-H stretching frequency increases from alkane → alkene → alkyne. Explain.
5. Show the formation of the peak at m/z = 94 in the mass spectrum of



6. Predict the number of signals and sketch the NMR spectrum of CH_3-O-CH_2-CH_2-Cl.
7. What are shift reagents in NMR spectroscopy? Explain.
8. How NMR spectroscopy is useful in distinguishing cis-stilbene and trans-stilbene?
9. Explain off resonance decoupling.
10. Explain the spin notation A_2X_3 in NMR spectroscopy with example.

(8 × 1 =8)

Section B

(Answer any **six** questions. Each question carries a weight of 2)

11. Explain the exchange phenomenon in ^{1}H NMR.

12. Discuss the effect of concentration on vibrational stretching frequency of methyl salicylate and ethanol.
13. A compound with molecular formula $C_4H_8O_3$ gave the following spectral data. Deduce the structure.

    IR: 1120, 1705 cm^{-1}

    ^1H NMR: δ 12.1(1H, s), 4.15(2H, s), 3.6(2H, q, J = 7 Hz) and 1.3(3H, t, J = 7 Hz) ppm
14. Write a note on HRMS and MS-MS.
15. Explain McLafferty rearrangement.
16. Discuss the technique - spectral editing based on DEPT.
17. Briefly explain cross polarization and selective population inversion in NMR spectroscopy.
18. A compound 'A' with molecular formula C_5H_{10} on ozonolysis gives 'B', C_4H_8O, as one of the products. The IR spectrum of B showed a band at 1720 cm^{-1} and the NMR spectrum showed three signals at δ values 0.9 (3H, t), 3.4 (2H, q) and 2.2 (3H, s). What are A and B? Explain.

(6 × 2 = 12)

Section C

(Answer any **two** questions. Each question carries a weight of 5)

19. Describe the following

    a) FAB b) MALDI c) Field desorption d) TOF e) Cyclotron
20. Predict the structure of the compound (MF $C_{11}H_{20}O_4$) which gave the following spectral data.

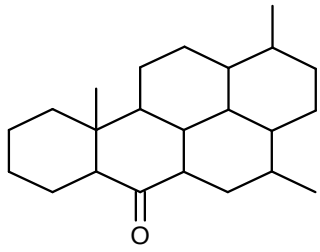
    UV – No λ_{max} above 200 nm IR: 1740 cm^{-1}.

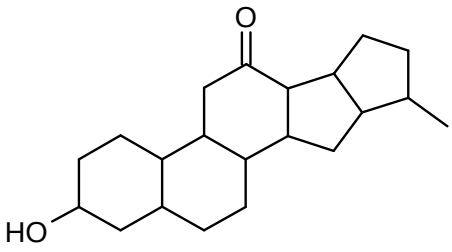
    ^{1}HNMR: δ 4.2 (4H, q), 3.3 (1H, t), 1.9 (2H, q), 1.33 (4H, m), 1.27 (6H, t) and 0.9 (3H, t) ppm.

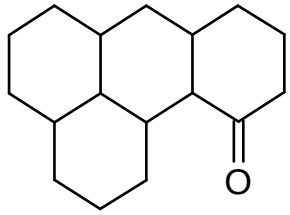
    ^{13}C NMR: δ 14.10, 13.81, 22.4, 28.5, 29.5, 52.0, 61.1 and 169.3 ppm.

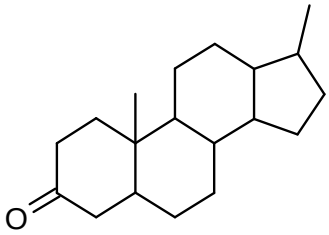
    Mass: m/z 216 ($M^{+\cdot}$), 171, 160 (100%), 133 and 115.
21. (a). Explain the magnetic anisotropy in carbonyl compounds and acetylene.

    (b). Define spin – spin coupling. Explain spin-spin coupling in the spin systems AX_2, AMX and ABC with examples.
22. Discuss Octant rule. Draw the octants for the following compounds and predict the sign of their optical activity.









(5 × 2 = 10)

QP Code **Reg. No. …..**

Name ……

M. Sc. Degree (C.S.S) Examination, 2019

Fourth Semester

Faculty of Science-Polymer Chemistry

CH 88 04 01 Properties and Characterisation Methods of Polymers

(2019 admissions onwards)

Time: Three hours Max. Weight: 30

Section- A

(Answer any **eight** questions. Each question carries a weight of 1)

1. Explain Hoffman's nucleation theory
2. What is Hildebrand solubility parameter? Give one of its applications
3. Define vicat softening temperature
4. Briefly explain the optical properties of polymers
5. How do you determine molecular weight by light scattering technique ?
6. What is cold drawing ?
7. How optical microscopy is used for morphological analysis ?
8. Define Deborah Number. What is its significance?
9. Describe fractionation of polymers by turbidimetric titration
10. Write the principle of gel permeation chromatography (GPC)

(8 x 1 = 8)

Section B

(Answer any **six** questions. Each question carries a weight of 2)

11. Discuss different methods for morphological analysis of crystalline polymers
12. Give a detailed description of polymer waste management
13. What are biodegradable polymers? Illustrate one test method to determine polymer biodegradability.
14. Demonstrate structure of spherulites and explain the relation of sherulites to crystallites
15. Write the mechanism of conduction in polymers and applications of conducting polymers
16. Describe Maxwell model for creep experiment

17. Write the principle of hardness test. Explain any two methods
18. How is fatigue test carried out?

(**6 x 2 = 12**)

Section C

(Answer any **two** questions. Each question carries a weight of 5.)

19. Give an account of conformations of polymer chain in solution
20. Discuss in detail the thermal and electrical properties of polymers
21. Explain the following characterisation methods: (a) differential scanning calorimetry (b) differential thermal analysis (c) thermo-mechanical analysis (d) thermo-gravimetric analysis
22. Explain Flory-Huggins theory and Flory-Krigbaum theory. Comment on advantages and limitations.

(**2 x 5 = 10**)

QP Code **Reg. No. …..**

Name ……

M. Sc. Degree (C.S.S) Examination, 2019

Fourth Semester

Faculty of Science-Polymer Chemistry

CH 88 04 02-Advances in Polymer Science and Technology

(2019 admissions onwards)

Time: Three hours Max. Weight: 30

Section A

(Answer any **eight** questions. Each question carries a weight of 1)

1. What are biomedical polymers? Analyse their importance with an illustrative example
2. Demonstrate electroluminescent polymers. Mention its relevance in the present day
3. Write the applications of conducting polymers using suitable example
4. Explain dunlop process
5. What is calendaring of polymers? Give two applications
6. How curving process is carried out?
7. What is VFA number ? How do you determine this value ?
8. What are XSBR and NBR lattices ? Explain their properties
9. Define *h*- index. What is its significance?
10. What is the process of vulcanization of rubber?

(8 x 1 = 8)

Section B

(Answer any **six** questions. Each question carries a weight of 2)

11. What are liquid crystalline polymers? Write the method of synthesis and applications.
12. Define composite. Explain properties and applications of nanoclay based composites
13. Write short essay on hazards and safety measures in paint industry
14. What do you mean by polymer blend? Outline their industrial applications
15. Differentiate between distributive mixing and laminar mixing
16. Demonstrate the various factors influencing the performance of polymer composites
17. Describe literature databases *viz.*, ScienceDirect, SciFinder, and Chemical Abstract
18. What are the various types of research possible in science?

(**6 x 2 = 12**)

Section C

(Answer any **two** questions. Each question carries a weight of 5)

19. Illustrate different types of adhesives and their applications
20. Differentiate between natural and man-made polymers. Write the synthetic approach towards (a) rayon (b) polyethylene terephthalate (c) nylon 6 and (d) nylon 66
21. Discuss various moulding processes of polymers
22. What is a polymer compound ? Write different types and characteristics of compound polymers

(2 x 5 = 10)

QP Code **Reg. No. …..**

Name ……

M. Sc. Degree (C.S.S) Examination, 2019

Fourth Semester

Faculty of Science-Polymer Chemistry

CH 88 04 03- Advanced Organic Chemistry

(2019 admissions onwards)

Time: Three hours Max. Weight: 30

Section- A

(Answer any **eight** questions. Each question carries a weight of 1)

1. What are cyclophanes ? Give an example
2. Define ionic liquid? Mention its advantages
3. What are selectrides ? Give their applications
4. How Nazarov cyclization is applied for the synthesis of five membered ring?
5. Comment on common protecting groups used in peptide synthesis
6. Write the mechanism of Swern oxidation
7. What is a dendrimer? Give the structure of a dendrimer as example
8. Point out the mechanistic difference between Prevost and Woodward reactions
9. Illustrate the enzymatic reduction using Baker's yeast. What is its advantage?
10. Suggest a method of preparation of lactone.

(8 x 1 = 8)

Section B

(Answer any **six** questions. Each question carries a weight of 2)

11. Give an account of the applications of supramolecular complexes in perfumery and medicine
12. Discuss the following: (a) coenzyme catalysed reactions (b) clay catalysed synthesis
13. Illustrate and compare the chromium based oxidation reactions: (a) John's oxidation, (b) Collin's oxidation (c) Sarrett oxidation
14. What is meant by multicomponent reactions? Explain the classic reactions (a) Ugi reaction (b) Passerini reaction (c) Biginelli reaction
15. Write the mechanism of Pauson-Khand reaction. Give two applications
16. What is DIBAL-H used for ? Discuss its mechanistic aspects

17. Describe the usefulness of the following reactions in organic synthesis: (a) Mitsunobu reaction (b) ozonolysis
18. Differentiate between Negishi and Sonogashira coupling reactions. Give one application for each reaction.

(**6 x 2 = 12**)

Section C

(Answer any **two** questions. Each question carries a weight of 5.)

19. Write the basic principles of retrosynthesis. Describe the retrosynthetic approach towards the preparation of D-luciferin
20. Explain the following metal based reductions: (a) Birch reduction (b) pinacol formation, (c) acyloin formation
21. Discuss in detail the various methods of inter conversion of ring systems (contraction and expansion procedure)
22. Write the general principles of microwave and ultrasound assisted organic synthesis

(**2 x 5 = 10)**