M.Sc

MASTER OF SCIENCE

IN

APPLIED CHEMISTRY

PROGRAM STRUCTURE AND SYLLABUS

2019-20 ADMISSIONS 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 **CH03 M.Sc APPLIED 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 Program 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 PG BoS 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 CoreGroup (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**
i.	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.

PROGRAM STRUCTURE

	Code	Courses	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 0203	Chemical Bonding and Computational Chemistry	4	72	3
	CH 50 0204	Molecular Spectroscopy	3	54	3
	CH 50 0205	Inorganic Chemistry Practical-1	3	54	3
	CH 50 0206	Organic Chemistry Practical-1	3	54	3
	CH 50 0207	Physical Chemistry Practical-1	4	72	3
		Total	**25**	**450**	**23**
Semester 3	CH 03 03 01	Essential Oils and Aromatics	4	72	4
	CH 03 03 02	Advanced Synthetic Organic Chemistry	4	72	4
	CH 03 03 03	Physical Chemistry	4	72	4
	CH 50 03 04	Spectroscopic Methods in Chemistry	3	54	4
	CH 03 0405	Industrial Oils and Fat Products Practical-1	3	54	Evaluation at the end of fourth semester
	CH 03 0406	Essential Oils and Aromatics Practical-2	3	54	
	CH 03 0407	Advanced Applied Chemistry Practical-3	4	72	
		Total	**25**	**450**	**16**

		Elective(Group A)			
Semester 4	CH 84 04 01	Industrial Oils and Fat Products	5	90	4
	CH 84 04 02	Biochemistry of Fatty Acids	5	90	4
	CH 84 04 03	Advanced Applied Chemistry	5	90	4
		Elective(GroupB)			
	CH 85 04 01	Advances in Polymer Science and Technology	5	90	4
	CH 85 04 02	Analytical Chemistry	5	90	4
	CH 85 04 03	Medicinal Chemistry	5	90	4
	CH 03 0404	Project			2
	CH 03 0405	Industrial Oils and Fat Products Practical-1	3	54	3
	CH 03 0406	Essential Oils and Aromatics Practical-2	3	54	3
	CH 02 0407	Advanced Applied Chemistry Practical-3	4	72	3
	CH 020408	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 dibenzene chromium, 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 COligands.

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, Bohr effect. 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 (9Hrs)

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 alkylidene cycloalkanes.

4.4 Topicity and prostereo isomerism, 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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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), Hermiteequation(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.

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

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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-Tiemann reaction. 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.
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4. J. March, M.B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6thEdn., Wiley, 2007.
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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 ofhelium 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, selfconsistent 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.

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

A) Molecular Mechanics:
Arguslab, Tinker, NAMD, DL-POLY, CHARMM, AMBER

B) Ab initio, semiempirical and dft:
1.Firefly / PC GAMESS available from http://classic.chem.msu.su/gran/gamess/
2.WINGAMESS available from http://www.msg.ameslab.gov/gamess/

C) Graphical User Interface (GUI):
1. Gabedit available from http://gabedit.sourceforge.net/
2.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)

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, 4thEdn., Tata McGraw Hill, 1994.
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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, 7thEdn., Longman,1996.
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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

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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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SEMESTER 3

CH 03 03 01 ESSENTIAL OILS AND AROMATICS

Credit 4 **Contact Hours: 72Hrs**

Objective of the Course

The learners should have an awareness about production,isolation and properties of essential oils and its constituents,spices and spice oils.

Unit 1: Essential oils (18 Hrs)

1.1 Production and isolation of essential oils: General methods for the production of essential oils, methods of isolation- hydro distillation, solvent extraction, enfleurage, maceration, expression, supercritical fluid extraction.

1.2 Sources, nature, chemical constituents, method of isolation and uses of the following essential oils: lemongrass oil, lemon oil, rosemary oil, camphor oil, eucalyptus oil, turpentine oil, jasmine oil, lavender oil, rose oil, sandal wood oil, clove oil, cinnamon oil, vetiver oil, peppermint oil.

Unit 2: Terpenoids (9 Hrs)

2.1 Introduction and classification of terpenoids, isoprene rule, general methods of determining structure.Biosynthesis of terpenoids: formation of mevalonic acid as intermediate. Biosynthesis of monoterpenoids and sesquiterpenoids.

Unit **3: Study of Essential oil constituents-I (18 Hrs)**

3.1 Natural sources, production, structure, properties, reactions and synthesis of thefollowing essential oil constituents.

Hydrocarbons: ocimene, α-pinene p-Cymene, Caryophyllene.

Alcohols: Geraniol, Citronellol, Terpineol, Menthol.

Aldehydes: Citral.

Ketones: Menthone, Pulegone, Camphor.

3.2 UV-visible, IR and mass spectral analysis of the following compounds: ocimene, α-pinene ,geraniol, citral, camphor.

Unit 4: Study of essential oil constituents- II (9 Hrs)

4.1 Natural source, production, structure, properties and uses of aromatics and essential oil constituents such as:

Alcohols: Cinnamyl alcohol, leaf alcohol

Aldehyde: Anisaldehyde, Vanillin.

Phenols: Eugenol, Isoeugenol, Methyl eugenol.

Esters: Cinnamyl acetate, Geranyl acetate, Linalyl acetate.

Misecellenous compounds : Coumarin, Muscone, Civetone, Artificial Musk.

Unit 5: Spices and spice oils (18 Hrs)

5.1 Sources, production, nature, chemical constituents and uses of the following spices: Cardamom, pepper, clove, nutmeg, mace, cinnamon, ginger, turmeric, coriander, garlic, vanilla, saffron, curry leaf and peppermint.

5.2 Spice oils and oleoresins - Methods of production, chemistry of the constituents and uses of the following spice oils and oleoresins- Pepper, ginger, turmeric.

References

1. F. Rosengarten, The Book of Spices, Jove, 1981.
2. J.W. Parry, Hand Book of Spices, Chemical Publishing, 1969.
3. J.S. Pruthi, Spices and Condiments Chemistry, Microbiology and Technology, Academic Press, 1980.
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5. L.H. Meyer, Food Chemistry, Reinhold, 1960.
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CH 03 03 02 ADVANCED SYNTHETIC ORGANIC CHEMISTRY

Credit:4 **Contact Hours : 72 Hrs**

Objective of the course

To understand the various organic reactions and reagents as tools for the synthesis of organic compounds. To learn the principles of retrosynthetic approach and supramolecular chemistry.

Unit 1: Asymmetric Synthesis (9 Hrs)

1.1 Stereoselectivity: Classification, terminology and principle.

1.2 Asymmetric synthesis and asymmetric induction- Double diastereoselection and double asymmetric induction- chiral auxiliaries and chiral pool

1.3 Assymetric aldol condensation pioneered by Evans.

1.4 Assymmetric Diels Alder reactions.

1.5 Enatioselective catalytic hydrogenation developed by Noyori

Unit 2 : Retrosynthetic Analysis and Construction of rings (18 Hrs)

2.1 Basic principles and terminology of reterosynthesis, important strategies of retrosynthesis, FGI, FGA, FGR, FGT. Synthesis of aromatic compounds- One group and two group C-X disconnection.

2.2 One group C-C disconnection:- Alcohols & Carbonyl compounds

Synthesis of amines and alkenes.Two group C-C disconnections:- 1,3 difunctionalised compounds & α,β – unsaturated carbonyl compounds. 1,5 – difucnationalised cpds-Michael addition & Robinson Annelation. Diels Alder reaction.

2.3 Different approaches towards the synthesis of three, four, five and six-membered rings. Photochemical approaches for the synthesis of four membered rings oxetanes and cyclobutanes, ketene cycloaddition (inter and intra molecular). Inter-conversion of ring systems (contraction and expansion)-Demjenov reaction

2.4 Cyclisation reactions: Pauson-Khand reaction, Volhardt reaction, Bergman cyclization, Nazarov cyclization

2.5 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.

2.6 Synthesis of some complex molecules using disconnection approach**:** (+) Heliotridine, Juvabione, luciferin

Unit 3: Organic Synthesis via Oxidation and Reduction (18 Hrs)

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

3.2 Survey of organic reagents and reactions in organic chemistry with special reference to reduction: (a) Catalytic hydrogenation (Heterogeneous: Pd /Pt /Rh /Ni; Homogeneous: Wilkinson), Noyori asymmetric hydrogenation (b) Metal based reductions using Li/Na/Ca in liquid ammonia, Sodium, Magnesium and Zinc (Birch, Pinacol formation, McMurry, Acyloin formation, dehalogenation and deoxygenations) (c) Hydride transfer reagents from Group III and Group IV in reductions (i) $NaBH_4$ triacetoxyborohydride; $LiAlH_4$ and DIBAL-H, Meerwein-Pondorff-Verley reduction) (ii) Stereo/enantioselective reductions (Chiral Boranes, Corey-Bakshi-Shibata).

Unit 4: Modern Synthetic Methods and Reagents (9 Hrs)

4.1 Baylis-Hillman reaction, Henry reaction, Nef reaction, Sakurai reaction, Tischenko reaction, Metal mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki, Negishi, Sonogashira, Nozaki-Hiyama, Buchwald-Hartwig, Ullmann and Glaser coupling reactions. Reagents such as: NBS, DDQ, DCC, Gilmann reagent.

4.2 Introduction to multicomponent reactions- Three component reactions (Mannich reaction, Passerini reaction, Biginelli reaction), Four component reactions (Ugi reaction). Click reactions (Elementary idea only).

Unit 5: Molecular Recognition and Supramolecular Chemistry (9 Hrs)

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

5.2 Molecular receptors: Cyclodextrins, Crown ethers, Cryptands, Spherands, Tweezers, Carcerands, Cyclophanes, Calixarenes, Carbon nanocapsules.

5.3 Importance of molecular recognition in biological systems like DNA and protein, Controlled release phenomena.

5.4 Applications of supramolecular complexes in medicine and perfumery industries.

Unit 6: Chemistry of Natural Products and Biomolecules (9 Hrs)

6.1 Synthesis of camphor, atropine, papavarine, quinine, cyanin, quercetin, β-carotene, testosterone, Vitamin A1.

6.2 Methods of primary structure determination of peptides, proteins and nucleic acids. Replication of DNA. Protein biosynthesis – transcription and translation, DNA sequencing. Polymerase chain reaction and human genome project.

References

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4. V.K. Ahluwalia, Oxidation in Organic Synthesis, CRC Press, 2012.
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CH 03 03 03 PHYSICAL CHEMISTRY

Credit: 4 **Total Hours: 72**

Objective of the course

To recognise the fundamental theories of reaction rates, mechanism of chain reactions, different types of surfaces, application of various isotherms in surface catalysed reactions, the excited states involved in photochemical reactionsand the kinetics of electrode reactions.

Unit 1: Chemical Kinetics and Catalysis (18 Hrs)

Absolute reaction rate theory(ARRT)-thermodynamic treatment, application of ARRT to simple bimolecular process- Mechanisms of Photochemical and Oscillatory Reactions -chain reactions – general characteristics- study of kinetics of chain reaction like H_2 -Br_2 reaction- decomposition of acetaldehyde and N_2O_5 ,study of H_2 - O_2 explosive reactions- Theory of unimolecular reactions-Lindemann- Hinshelwood, RRKM and Slater treatment- steady state approximation, principle of microscopic reversibility and detailed balancing - kinetic isotope effect- primary and secondary kinetic salt effect- influence of solvent on reaction rates - Significance of volume and entropy of activation- Study of fast reactions by Stopped flow method-Specific and general acid-base catalysis- Bronsted catalysis law- Acidity functions- Enzyme catalysis (single substrate reactions only).Michaelis-Menton kinetics.- Influence of pH and temperature on enzyme catalysis- Kinetics of heterogeneous catalysis (Langmuir Hinshelwood mechanism and Eley-Rideal mechanism)

Unit 2: Surface chemistry (18 Hrs)

Different types of surfaces-thermodynamics of surfaces- Adsorption isotherms- Freundlich – Langmuir isotherm and derivation-BET theory and kinetic derivation- surface area determination-Temkin adsorption isotherm-Adsorption on liquid surface-surface tension- Gibbs's adsorption isotherm- Application of Langmuir adsorption isotherm in surface catalysed reactions- the Eley-Rideal mechanism and the Langmuir-Hinshelwood mechanism, flash desorption- Colloids: Zeta potential- electrokinetic phenomena- sedimentation potential and streaming potential- Donnan membrane equilibrium- Surface Enhanced Raman Scattering, surfaces for SERS studies- Experimental methods of studying surfaces - Augar, LEED and ESCA.

Unit 3: Electrochemistry (22Hrs)

Theories of ions in solution- Drude and Nernst's electrostriction model and Born's model Mechanism of electrolytic conductance, relaxation and electrophoretic effects, Debye – Huckel – Onsager (DHO) equation and its validity in aqueous and non -aqueous solutions. Deviations from the Onsager equation, conductance ratio and Onsager equation. Dispersion of conductance at high frequencies (Debye – Falkenhagen effect).Conductance with high potential gradients (Wien effect).Activity and activity coefficient, forms of activity coefficients, activities of electrolytes and mean ion activity coefficient.The Debye – Huckel

Limiting law.Electrokinetic phenomena: Electrical double layer and its structure (Stern's theory), Electroosmosis, Streaming potential, Electrophoresis, Influence of ions on electrokinetic phenomena- Principles and applications of Cyclic voltammetry- Principles and Applications of impedance measurements- Electrode modification- Fluorescence, chemi and bio-luminescence sensors-Fluorescent tag molecules- Applications- Conductometric sensors- Coulometric sensors- Voltammetric sensors- Amperometric sensors- Neurotransmitters- Applications

Unit 4: Photochemistry (14 Hrs)

Photophysical processes of electronically excited molecules- Franck – Condon principle– quantum mechanical treatment-Dissociation and pre – dissociation of diatomic molecules- Energy transfer from electronically excited molecules- Stern – Volmer mechanism only- Photophysical pathways: fluorescence, phosphorescence, E-type and P- type delayed fluorescence. Kinetic treatment of excimer and exciplex formation- lasers in photochemical kinetics-Photochemical splitting of water- organic light emitting devices.

References

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20. West,A. R.Solid state chemistry and its applications, Wiley Publishers.

CH 50 03 04 SPECTROSCOPIC METHODS IN CHEMISTRY

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

Objective of the Course

The learners should be able to apply the different spectroscopic methods to solve problems based on it, to apply spectral data for explaining important organic reactions and functional transformations

Unit 1: Ultraviolet-Visible and Chiro-optical 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. Chiro-optical 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 ^{1}H and ^{13}C nuclei. Chemical shift and shielding/deshielding, factors affecting chemical shift, relaxation processes, chemical and magnetic non-equivalence, local diamagnetic shielding and magnetic anisotropy. ^{1}H and ^{13}C NMR scales.

3.2 Spin-spin splitting: AX, AX_2, AX_3, A_2X_3, AB, ABC, AMX type coupling, first order and non-first order spectra, Pascal's triangle, coupling constant, mechanism of coupling- 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, ^{1}H NMR and ^{13}C NMR spectroscopy (HRMS data or Molar mass or molecular formula may be given).

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

5.3 Spectral analysis of the following reactions/functional transformations:

1. Pinacol-Pinacolone rearrangement
2. Benzoin condensation
3. (4+2) cycloaddition
4. Beckmann rearrangement
5. Cis-trans isomerisation of azo compounds
6. Benzil-benzilic acid rearrangement
7. 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

CH 84 04 01 INDUSTRIAL OILS AND FAT PRODUCTS

Credit 4 **Lecture Hours : 90 Hrs**

Objective of the course

To have a well organised knowledge about extraction and processing of oils and fats

Unit 1: Extraction and Processing of Oils and Fats (18 Hrs)

1.1. Mechanical pretreatment and heat treatment of oil bearing materials. Rendering of animal fats and cooking of oil seeds. Mechanical expression of oils. Solvent extraction-theory and practice, type of extractors, solvent recovery, alternative solvents for extraction, super critical fluid extraction of oils and fats.

1.2. Refining, bleaching, deodorization, fractionation, winterization, stabilization, solidification, homogenization, emulsification and dewaxing.

1.3 Study of the sources, composition, characteristics and utilization of commercially

important oils and fats- butter, tallow, coconut oil, palm oil, cocoa butter, olive oil, rice bran oil, sesame oil, soybean oil, sunflower oil, linseed oil, mustard oil, castor oil.

Unit 2:Oilsand Fats as Food Materials (9 Hrs)

2.1 Cooking oil, salad oil, and salad dressings. Quality evaluation of cooking oils and salad oils. Margarine and Shortenings

2.2 Essential fatty acids: ω-3 and ω-6 fatty acids and their dietary sources, significance to human nutrition and health.

2.3 Fat-related diseases: atherosclerosis, arthritis. Nutritional significance of EFA, HDL, LDL and VLDL.

Unit 3:Hydrogenation of Oils (9 Hrs)

Catalytic hydrogenation: chemistry of hydrogenation, hydrogenolysis, influence of various factors in hydrogenation, mechanism, kinetics and thermodynamics of hydrogenation reactions, hydrogenation catalysts-theory of catalysis

Manufacture of catalyst for hydrogenation-Hydrogenation of vegetable and marine oils-manufacture of vanaspati

Unit 4:Fat Splitting and Esterification (**18 Hrs)**

4.1 Fat splitting: Twitchell process- low pressure splitting with catalysts, medium pressure autoclave splitting with catalyst, continuous uncatalysed high pressure counter current splitting, enzymatic splitiing, recovery of glycerine from fat splitting process and spent lye, different grades of glycerine, chemistry and synthesis of glycerine, uses of glycerine, glycerine substitutes.

4.2. Esterification: mechanism of esterification and ester hydrolysis, esterification of fatty acids with glycerol and other alcohols, inter esterification, acidolysis alcoholysis, glycolysis, glycerolysis, transesterification and its mechanism, applications of esterification and inter esterification

Unit 5: Rancidity in Oils, Fats and Oil Bearing Substances (**9 Hrs)**

Concept of autoxidation, theories of autoxidation, tests for rancidity, stability of oils, induction period, Pro oxidants and antioxidants, drying, semidrying and non-drying oils

Unit 6: Analysis of Fats and Oils (**18 Hrs)**

6.1 Test methods for physical properties: melting point, softening point, slipping point, titer, congeal point, flow test, cloud test, consistency test, penetration method, liquid and solid fatty acid determination, solid fat index, specific gravity, refractive index, viscosity, color, odor.

6.2 Test methods for chemical properties: Iodine value, thiocyanogen number, saponification value, acid value and free fatty acid, oxirane oxygen, hydroxyl andacetyl value, peroxide value, Reichert-Meissel value, Polenski value and Kirschner value, diene value. Estimation of poly unsaturated fatty acids-Kries test, thiobarbituric acid test

6.3 Adulteration of oils fats – detection of adulteration

Unit 7: Waxes and Fatty alcohols (**9 Hrs)**

7.1 Occurrence, classification, properties and composition of waxes. Synthetic waxes.Analysis and utilization of waxes.

7.2 Naturally occurring fatty alcohols – production, uses and applications Alcohol ethers.

References

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3. E.S. Pattison, Fatty acids and their Industrial Applications,Marcel Dekker, 1968
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CH 84 04 02 BIOCHEMISTRY OF FATTY ACIDS

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

Objective of the course

The learners should have a knowledge about source and classification of oils and fats,methods of isolation ,classification and properties of fatty acids

Unit 1: Lipids (9 Hrs)

1.1 Classification of lipids-sources and classification of oils and fats, nomenclature of triglycerides, stereospecific numbering

1.2 Nutritional functions of fats and oils, Caloric and non-caloric functions, Non nutritional functions of edible fats.

Unit 2: Glyceride structure (9 Hrs)

2.1 Glyceride composition of natural fats. Methods of investigation of glycerides.Theories of glyceride structure

Unit 3: Nonglyceride constituents of fats and oils (9 Hrs)

3.1 Occurrence, chemistry and function of carotenes, vitamins, tocopheols, steroids, phospholipids, sphingolipids, antioxidants. Constituents contributing flavor and odor.

Unit 4: Isolation and Characterization of Fatty Acids (9 Hrs)

4.1 Crystallisation methods, Chromatographic techniques: TLC, paper chromatography, GLC, HPLC. Use of IR, UV, NMR and mass spectrometry.

4.2 Nomenclature of fatty acids- IUPAC and omega reference systems, uses of fatty acids in textiles, leather, pharmaceuticals and petroleum processing.

Unit 5: Fatty Acids Occurring in Nature (18 Hrs)

5.1 Saturated fatty acids: important sources, structure and synthesis of naturally occurring straight chain and branched chain saturated fatty acids.

5.2 Unsaturated fatty acids: mono ethenoid fatty acids-their occurrence and general methods of synthesis. Oleic acid and petroselenic acid-properties and constitution.

5.3 Polyunsaturated fatty acids, cyclopropenoid acids, conjugated acids, epoxy acids, keto acids, cyclopentenoid acids, hydroxy acids, acetylenic acids, furanoid acids, artificially produced fatty acids.

Unit 6: Physical properties of Fatty Acids (9 Hrs)

6.1 Crystal properties, thermal properties, spectral properties, solubility and solution properties of fatty acids in the liquid state.

Unit 7: Chemical properties of Fatty Acids (**18 Hrs)**

7.1 Salt formation, esterification, halogenation, oxidation uses of various oxidizing agents like chromic acid, ozone, peroxides, potassium permanganate, periodic acid and lead tetra acetate. Hydrogenation, dehydration, pyrolysis, polymerization, addition reactions to double bond.

Unit 8: Biochemistry and Metabolism of Fats **(9 Hrs)**

8.1 Biochemical transformation of fats in the body-biosynthesis of fats in plants and animal organisms.

8.2 Prostaglandins: synthesis, biosynthesis, applications of prostaglandins as drugs.

References

1. M.G. Wohl, R.S. Goodhart, M.E. Shils, Modern Nutrition in Health and Disease, 6thEdn., Lea & Febiger, 1980.
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CH 84 04 03 ADVANCED APPLIED CHEMISTRY

Credit 4 **Contact Lecture Hours: 90**

Objective of the course

To study the different types of soaps and detergents, paints and varnishes, drugs and their mode of action

Unit 1: Soaps and Detergents (18 Hrs)

1.1 Theory of surface action. Soap manufacture: raw materials, characteristics of cold process, semi boiled process and boiled process, additives of soap, detergent action of soap, influence of fatty acid composition of the oil on properties of soap, manufacture of soap for different purposes-laundry soaps, toilet soaps, liquid soaps, transparent soaps, baby soaps, shaving soaps, medicated soaps, textile soaps, naphtha soaps, marine soaps. T.F.M value of soaps, Shampoos.

1.2 Anionic, cationic, amphoteric and nonionic detergents used in modern industries and for household purposes-their chemistry, manufacture and applications- Agglomeration. Merits and demerits of syndets over soaps, biodegradability of detergents Role of surfactants in synthesis of nano particles, enzyme detergents, Green detergents, compact detergents

Unit 2: Paints and Varnishes (9 Hrs)

2.1 Paints as protective coatings, paints and enamels, materials for paint manufacture, oils used-unmodified oils and their pretreatment, modified drying oils, resins and copolymers-natural resins, phenolic resins, alkyd resins, urethane resins, epoxy resins-Driers, thinners, pigments and miscellaneous ingredients, mechanism of polymerization and drying of oils-Varnishes and lacquers: composition and uses, oleoresinous varnishes, defects in varnish films.

Unit 3: Flavour and Perfume Chemistry (18 hrs)

3.1 Concept of flavor, difference between perfumes and flavour. Flavour Characterisation.

3.2 Sensory analysis-descriptive and discriminent Sensory Analysis.

3.3 Flavour of Coffee, Tea, Cocoa, Onion and Garlic. Synthetic ingredients of food flavourings.

3.4 Odour, Odorants, Olfaction, Classification of odour. General Physiology of Olfaction.

3.5 Perfume Raw materials-Terpeneless and sesquiterpeneless oils, Concrete oils, Absolute oils, Isolates from essential oils, Tincture, Balsams and Resins.

3.6 Source and Chemical nature of commercially important Gums(Gum Arabic, Gum Tragacanth, Karaya Gum, British gum, Gum Myrrh), Balsams (Balsam of Peru,

Balsam of Tolu, Styrax) and Resins (Copals, Turpentines, Dragon's Blood, Damars, Amber, Lacquer, Shellac, Kinos, Asafetida)

3.7 Perfume Technology-blending and formulation of perfumes. Aerosol Spray Perfumes

Unit 4: Drug Chemistry and Phytochemicals (18 Hrs)

4.1. General Principles of Drug Therapy.Relationship between chemical structure, lipid solubility and biological activity of drugs.Stereochemistry and biological activity.

4.2. Antibiotics: Cell wall biosynthesis, inhibitors, β-lactum rings, antibiotics inhibiting protein synthesis. Synthesis of Penicillin G, Chloramphenicol and streptomycin.

4.3. Phytochemicals: Introduction to phytochemistry, Common phytochemicals and chemical defence, Importance and applications of phytochemicals in pharmacology.

Unit 5: Dairy Chemistry (9Hrs)

5.1 Milk :Definition,general composition of milk , constituents of milk - lipids, proteins, carbohydrates ,vitamins and minerals ,physical properties of milk - colour, odour, acidity, specific gravity, viscosity and conductivity.

5.2 Factors affecting the composition of milk :Adulterants, preservatives and neutraliser-examples and their detection, estimation of fat, acidity and total solids in milk.

5.3 Processing of Milk: Destruction of microorganisms in milk ,physico - chemical changes taking place in milk due to processing - boiling, pasteurisation , types of pasteurisation - Bottle, Batch and HTST (High Temperature Short Time) - Vacuum pasteurisation - Ultra High Temperature Pasteurisation.

5.4 Milk products: Cream, definition, composition,chemistry of creaming process, gravitational and centrifugal methods of separation of cream, estimation of fat in cream. Butter : definition , composition , theory of churning , estimation of acidity and moisture content in butter. Ghee :major constitutents, common adulterants added to ghee and their detection.

Unit 6: Green Chemistry (9 Hrs)

6.1. Principles of green chemistry, basic concepts, atom economy, twelve laws of green chemistry, principles of green organic synthesis, Green solvents: Ionic liquids, supercritical CO_2, fluorous chemistry.

6.2. Green alternatives of organic synthesis: Condensation reactions like aldol condensation & Benzoin condensation , oxidation reactions like Baeyer- Villiger oxidation & oxidation of ethyl alcohol to acetic acid, reduction reactions like Clemmensen reduction & reduction of carbonyl compounds, rearrangement reactions like pinacol- pinacolone rearrangement &benzil- benzilic acid rearrangement,

coenzyme catalysed reactions like oxidation of primary alkyl halide to carboxylic acid & oxidation of primary amine to carboxylic acid, clay catalysed reactions like Beckmann rearrangement & oxidation of alcohol to carboxylic acid, microwave assisted reactions like Cannizzaro reaction & Wittig reaction, green photochemical reactions like photo reduction of benzophenone to benzopinacol & Paterno- Buchi reaction

Unit 7: Nanotechnology (9 Hrs)

7.1. Basic principles of nanochemistry. Types of nanomaterials :Carbon nanotubes, fullerenes, quantum dots, nanowires, nanocones, haeckelites, graphenes and metal nanoparticles

7.2. Brownian motion, surface forces, self-assembly.General methods of synthesis of nanomaterials:Top-down production, bottom-up production. (Any two methods)

7.3 Applications of nanomaterials in medicine: Immunogold labeling, applications in medical diagnosis, nano based drug delivery, biomimetic nanotechnology, DNA nanotechnology

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GROUP B

CH 85 04 01 ADVANCES IN POLYMER SCIENCE AND TECHNOLOGY

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

Objective of the Course

To have a well organised knowledge about speciality polymers,polymer blends and composites, polymer mixing and compounding, adhesives,techniques of surface coating and to have an idea about fibre science and technology

Unit 1: Speciality Polymers (18Hrs)

1.1 Poly electrolytes: The 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 (12Hrs)

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.

2.3. 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.

3.2 Compatibility of blends: Principles of solubility and compatibility, thermodynamics of miscibility, mechanical compatibility.

3.3 Phase morphology: Phase separation behaviour, morphology of blends and its determination- electron microscopy- domain structure.

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

3.5. Industrial applications of polymer blends.

3.6. 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.,

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

3.8. 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, advantages and disadvantages of each method.

3.9. Nano-composites: Definition, types, methods of fabrication, characterization, uses and applications.

Unit 4: Polymer Compounding and Processing (18Hrs)

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, scale of segregation and intensity of segregation, 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, filler reinforcement, 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.

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, calendering

Unit 5: Fibre Science and Technology (12 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, acrylics, 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: Latex Technology (12 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 types and 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.

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CH 85 04 02 ANALYTICAL CHEMISTRY

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

Objective of the Course

To analyse and apply various instrumental methods and analytical procedures to molecular systems. To have an idea about renewable and non renewable aquatic resources

Unit 1: Instrumental Methods (36 Hrs)

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

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

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

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

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

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

1.7 Raman spectrometric instrumentation: Sources, sample illumination systems. Application of Raman Spectroscopy in inorganic, organic, biological and quantitative analysis.

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

Unit 2: Sampling (18 hrs)

2.1 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, electro dialysis, 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.

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CH 85 04 03 MEDICINAL CHEMISTRY

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

Objective of the Course

To study the different types of drugs and their mode of action in biological systems

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, H_1 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.

References

1. G.L. Patrick, Medicinal Chemistry, BIOS, 2001.
2. T. Nogrady, D.F. Weaver, Medicinal Chemistry, Oxford University Press, 2005.
3. W.O. Foye, T.L. Lemke, D.A. Williams, Principles of Medicinal Chemistry, 4thEdn., Williams & Wilkins, 1995.
4. J.P. Remington, Remington's Pharmaceutical Sciences, Vol.13, 19th Edn., Mack, 1990.
5. D. Sriram, P.Yogeswari, Medicinal Chemistry, Pearson Education India, 2010.
6. K.D. Tripathi, Essentials of medical Pharmacology, 6thEdn., Jaypee, 2008
7. L.S. Goodman, A. Gillman, The Pharmacological Basis of Therapeutics, 10th Edn., McGraw Hill, 2001.
8. S.S. Kadam, Principles of Medicinal Chemistry, Vol.I & II, Pragati Books, 2008.
9. A. Kar, Medicinal Chemistry, New Age International, 2007.
10. C.O. Wilson, J.M. Beale, J. Block, Textbook of Organic Medicinal and Pharmaceutical Chemistry, 12th Edn., Lippincott Williams and Wilkins, 2010.

SEMESTERS 3 AND 4

CH 03 04 05 INDUSTRIAL OILS AND FAT PRODUCTS - PRACTICAL I

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

I. Analysis of Vanaspati:

1. Determination of the physical and chemical constants of hydrogenated fats.
2. Estimation of Vitamin A and Vitamin E content of Vanaspati.
3. Detection of animal fats in Vanaspati.
4. Estimation of nickel in catalyst mixture and spent catalyst.

II. Soap analysis:

1. Complete analysis of washing soaps, toilet soaps and transparent soaps: Moisture, alcohol soluble and insoluble's, free caustic alkali, combined alkali, anhydrous soap, titer, mean molecular weight and Iodine value of total fatty acids derived from soaps.
2. TFM value of toilet soaps.
3. Estimation of glycerine content of toilet soaps and transparent soaps.
4. Test for detection of rosin in soaps. Estimation of rosin in soaps.

III. Estimation of Glycerol:

Estimation of glycerol in the given sample.

IV. Preparation of different types of soaps:

a) Washing soap, toilet soap, transparent soap, liquid soap, shaving soap.

b) Preparation detergent powder, shampoo, vanishing cream.

References

[1] F. Shahidi, Bailey's Industial Oil and Fat Products, 6th Edn., John Wiley & Sons, 2005.

[2] I. Ash, M. Ash, Formulary of Detergents and other Cleaning Agents, Chemical Publishing, 1999.

[3] H. Butler, Poucher's Perfumes, Cosmetics and Soaps, 10thEdn., Springer, 2000.

CH 03 04 06 ESSENTIAL OILS AND AROMATICS - PRACTICAL II

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

I. Extraction of some essential oils

Lemongrass oil, cinnamon oil, clove oil

II. Preparation of citral from lemongrassoil, cinnamaldehyde from cinnamon oil, eugenol from clove oil

III. Assay of essential oils and perfumery materials:

1. Determination of specific gravity, refractive index, optical rotation, boiling point and boiling range. Fractionation and solubility.
2. Estimation of essential oil constituents such as alcohols, esters, aldehydes, ketones, phenols and others.

Examples-

1. Estimation of acids in essential oils.

2. Geraniol in palmarosa oil.

3. Citronellol in citronella oil.

4. Linalool in bergamot or lavender oil.

5. Citral in lemongrass oil.

6. Citronellal in citronella oil.

7. Cinnamic aldehyde in cinnamon oil.

8. Methyl salicylate in wintergreen oil.

9. Geranyl acetate in palmarosa oil.

10. Camphor in camphor oil.

11. Cineole in eucalyptus oil.

12. Eugenol in clove oil.

13. Estimation of vanillin.

14. Estimation of aldehydes and ketone components in a mixtrure.

IV. Detection and estimation of common adulterants

Alcohol, rosin, fatty oil and mineral oil in essential oils.

V. Preparation of some typical isolates from essential oils.

1. Citral from lemongrass oil.

2. Cineol from eucalyptus oil.

3. Cinnamic aldehyde from cinnamon oil.

4. Eugenol from clove oil.

VI. Synthesis and spectral analysis of aromatics and perfumery compounds:

Synthesis and spectral analysis of aromatics and perfumery compounds by conventional method/Green method and spectral analysis by FTIR and NMR

1. Nerolin.

2. B- ionone.

3. Methyl heptenone.

4. Camphor.

5. Methyl cinnamate.

6. Methyl anthranilate.

7. Benzyl acetate.

8. Amyl benzoate.

9. Coumarin.

10. Amyl salicylate

References

1. E. Guenther, The Essential Oils-Vol.1, Jepson Press, 2007.

2. W.A. Poucher, Perfumes, Cosmetics and Soaps, 9th Edn., Springer, 1993.

3. M. Billot, F.V. Wells, Perfumery Technology: Art, Science, Industry, E. Horwood, 1975.

4. J.S. Pruthi, Spices and Condiments: Chemistry, Microbiology, Technology, Academic Press, 1980.

5. R.F. Venn, Principles and Practice of Bioanalysis, Taylor& Francis, 2007.

6. G. Reineccius, Flavour Chemistry and Technology, 2nd Edn., 2005.

7. V.C. Mehlenbacher, Official and Tentative Methods of the American Oil Chemists Society Vol.1, 3rd Edn., The Society, 1954.

8. H.A. Boekenoogen, Analysis and Characterization of Oils, Fats and Fat Products, Interscience, 1954

9. V.K. Ahluwalia, Green Chemistry: Environmentally Benign Reactions, Ane Books, 2009.

10. Monograph on Green Chemistry Laboratory Experiments, Green Chemistry Task Force Committee, DST, 2009.

11. R. M. Silverstein, F. X. Webster, D. J. Kiemle, D. L. Bryce, Spectroscopic Identification of Organic Compounds, 8th Edn., Wiley, 2015.

12. F. G. Mann and B.C. Saunders, Practical Organic Chemistry, Pearson.

13. J. B. Cohen, Practical Organic Chemistry, McGraw Hill.

CH 03 04 07 ADVANCED APPLIED CHEMISTRY - PRACTICAL III

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

I. Determination of the physical and chemical constants of common oils and fats

Moisture, Specific gravity, Refractive index, Acid value and free fatty acid, Saponification value, Iodine value, Non-saponifiable matter, Acetyl and hydroxyl value, Reichert Meissl value, Polenske and Kirschner value, peroxide value and color measurement of the following:

Coconut oil, Sesame oil, Palm oil, Olive oil, Castor oil, Ghee, Tallow

II. Milk and milk product analysis

1. Detection of starch inmilk

2. Detection of formalin in milk

3. Estimation of added glucose in milk

4. Estimation of starch in milk

5. Determination of total solids in milk

6. Determination of fat in milk

III. Ghee analysis

1. Determination of moisture in ghee

2. Determination of free fatty acids in ghee

3. Detection of vanaspathi in ghee

4. Determination of RM and Polenske-values of ghee

IV. Water analysis

Determination of P^H, TS, DO, TDS, COD, Hardness, Alkalinity, Chloride, Conductance etc. of water.

V. Simple experiments in Drug Chemistry

Preparation of aspirin, Preparation of paracetamol

VI. Colorimetric estimation of cholesterol in fats.

VII. Preparation of rice bran oil by solvent extraction method.

VIII. Preparation based on oils and fats

Preparations involving epoxidation, hydroxylation, bromination and chain scission of fatty acids.Isolation of individual fatty acids from oils.

1. Epoxystearic acids, 2. Erythro-9, 10-dihydroxystearic acid, 3.Threo-9, 10dihydroxystearic acid. 4. Tetrabromostearic acid. 5. Azelaic acid. 6. Sebacic acid. 7. Undecylenic acid. 8. Isolation of palmitic acid from palm oil. 9. Isolation of erucic acid from mustard oil.

References

1 V.C. Mehlenbacher, Official and Tentative Methods of the American Oil Chemists Society Vol.1, 3rd Edn., The Society, 1954.

2. H.A. Boekenoogen, Analysis and Characterization of Oils, Fats and Fat Products, Interscience, 1954.

3. L.V. Cocks, C.V. Rede, Laboratory Hand Book for Oil and Fat Analysis, Academic Press, 1966.

4. F.D. Gunstone, An Introduction to the Chemistry and Biochemistry of Fatty Acids and their Glycerides, Chapman and Hall, 1968.

5. F.D. Gunstone, Topics in Lipid Chemistry, Logos, 1970.

6. AOCS (American Oil Chemists' Society)

7. N. P. Wong, R. Jenness, M. Keeney and E. H. Marth, Fundamentals of diary chemistry, Springer, 1988.

8. D. D. Roy, P. Dinakar and M. P. Mathur, Text book of diary chemistry, Indian council of agricultural, 2008

9. M. Zaffer Ahmad and Muhammed Ali, Text book of pharmaceutical drug analysis, CBS publishers, 2009.

10. Ashutosh Kar, Pharmaceutical drug analysis, New Age International Pvt. Ltd., 2005.

MODEL QUESTION PAPERS

QP Code **Reg. No. …..**

Name ……

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

First Semester

Faculty of Science- Chemistry

CH03 Applied 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
CH03 Applied Chemistry

CH 50 01 02 STRUCTURAL AND MOLECULAR ORGANIC CHEMISTRY
(Common forall 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

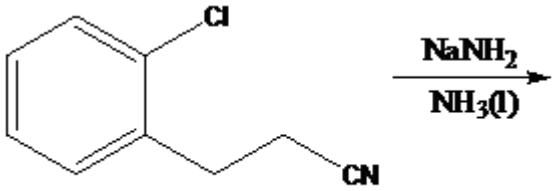
(Answer any **six** questions. Each question carries a weight of 2)

11. Predict the product and explain the mechanism

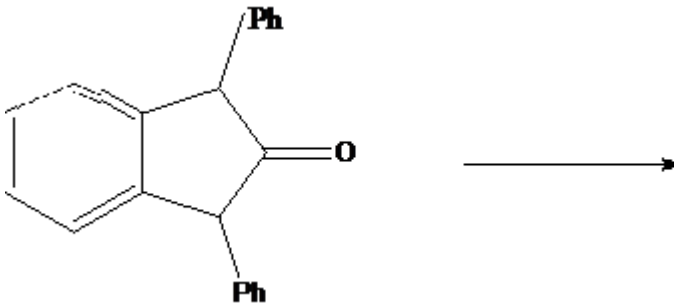
(Answer any **six** questions. Each question carries a weight of 2)

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.

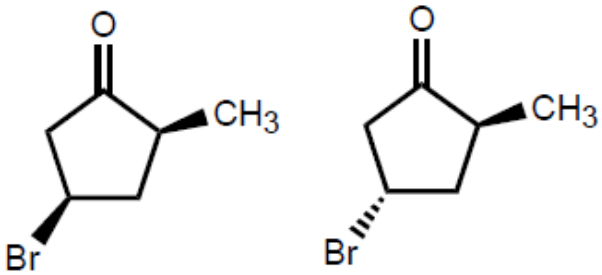
14.What are hard and soft acids? Use HSAB principle to distinguish them

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 Chemistry Degree(C.S.S) Examination, 2019

First Semester

Faculty of Science- Chemistry

CH03 Applied Chemistry

CH 50 01 03-Quantum Chemistry and Group Theory

(Common for all branches of Chemistry)

(2019 admissions onwards)

Time: Threehours **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 what are 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 $\Psi(x,y,z) = (8/abc)^{1/2}$ $(sinnx\Pi x/a)$ $(sinny\Pi y/b)(sinnz\Pi z/c)$ 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, ……

First Semester

Faculty of Science- Chemistry

CH03 Applied 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 $25^{o}C$ and

–83.68 kJ at 35^{o}C. Calculate the change in enthalpy (ΔH) for the process at 30^{o}C.

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 4.59×10^{-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 Chemistry Degree (C.S.S) Examination, ……

Second Semester

Faculty of Science- Chemistry

CH03 Applied Chemistry

CH 50 02 01 - COORDINATION 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 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 d^9 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

Second Semester

Faculty of Science- Chemistry

CH03 Applied Chemistry

CH500202- 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 importances 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 importances 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. ScChemistry Degree(C.S.S) Examination, 2019

Second Semester

Faculty of Science- Chemistry

CH03 Applied 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)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 Chemistry Degree (C.S.S) Examination, ……

Second Semester

Faculty of Science- Chemistry

CH03 Applied 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)**