M.Sc

MASTER OF SCIENCE

IN

PHRMACEUTICALCHEMISTRY

PROGRAM STRUCTURE AND SYLLABUS

2019-20 ADMISSION ONWARDS

(UNDER MAHATMA GANDHI UNIVERSITY PGCSS REGULATIONS 2019)

BOARD OF STUDIES IN CHEMISTRY (PG)

MAHATMA GANDHI UNIVERSITY

2019

PREFACE

I feel privileged in presenting the revised curriculum and syllabus of **CH04 M.Sc PHARMACEUTICAL CHEMISTRY PROGRAM** for favour of approval by the Faculty of Science and Academic Council of Mahatma Gandhi University, Kottayam, Kerala, India.

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

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

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

Dr.GEETHA P

Chairperson, PG Board of Studies in Chemistry

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M.Sc Degree Program-CH 04 Pharmaceutical Chemistry

(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 thanCCPA 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 requirementfor admission
2. For OEC categoryCCPA of 4.5in the qualifying examination is required

3. Medium of instruction

English

4.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 and150respectively.

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 390hours stipulated by the UGC.

PROGRAM STRUCTURE

	Code	Courses	Hours / Week	Total Hours	Credit
Semester 1	CH 50 01 01	Organometallics and NuclearChemistry	4	72	4
	CH 50 01 02	Structural and Molecular Organic Chemistry	4	72	4
	CH 50 01 03	Quantum Chemistry and Group Theory	4	72	4
	CH 50 01 04	Thermodynamics, Kinetic Theory and Statistical Thermodynamics	3	54	4
	CH 50 02 05	Inorganic Chemistry Practical-1	3	54	Evaluation at the end of second semester
	CH 50 02 06	Organic Chemistry Practical-1	3	54	
	CH 50 02 07	Physical Chemistry Practical-1	4	72	
		Total	**25**	**450**	**16**
Semester 2	CH 50 02 01	Coordination Chemistry	4	72	4
	CH 50 02 02	Organic Reaction Mechanisms	4	72	4
	CH 50 02 03	Chemical Bonding and Computational Chemistry	4	72	3
	CH 50 02 04	Molecular Spectroscopy	3	54	3
	CH 50 02 05	Inorganic Chemistry Practical-1	3	54	3
	CH 50 02 06	Organic Chemistry Practical-1	3	54	3
	CH 50 02 07	Physical Chemistry Practical-1	4	72	3
		Total	**25**	**450**	**23**
Semester 3	CH 04 03 01	Synthetic and Bioinorganic Chemistry	4	72	4
	CH 04 03 02	Physical Chemistry	4	72	4
	CH 04 03 03	Drug Design and Pharmacology	4	72	4
	CH 50 03 04	Spectroscopic Methods in Chemistry	4	54	4
	CH 04 04 05	Pharmaceutical Analysis Practical	3	54	Evaluation

	CH 04 04 06	Drug Synthesis and Dispensing Practical	3	54	at the end of
					fourth semester
	CH 04 04 07	Biochemistry and Bacteriology Practical	4	72	
		Total	**25**	**450**	**16**
		Elective(Group A)			
Semester 4	CH 86 04 01	Bacteriology and Biochemistry	5	90	4
	CH 86 04 02	Advanced Pharmaceutical Operations and Dispensing	5	90	4
	CH 86 04 03	Medicinal Chemistry	5	90	4
		Elective(Group B)			
	CH 87 04 01	Advanced Organic Chemistry	5	90	4
	CH 87 04 02	Advanced Pharmaceutical Operations and Dispensing	5	90	4
	CH 87 04 03	Industrial Oils and Fat Products	5	90	4
	CH 03 04 04	Project			2
	CH 04 04 05	Pharmaceutical Analysis Practical	3	54	3
	CH 04 04 06	Drug Synthesis and Dispensing Practical	3	54	3
	CH 04 04 07	Biochemistry and Bacteriology Practical	4	72	3
	CH 0204 08	Viva			2
		Total	**25**	**450**	**25**
Grand Total					**80**

SEMESTER 1

CH 50 01 01 ORGANOMETALLICS AND NUCLEAR CHEMISTRY

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

Objective of the course

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

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

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. Radicaltype reactions, electrophilic reactions, carbonylation and borylation of arenes.Insertion of alkenes and alkynes in the Ar-H bond.

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

Unit 4: Bioinorganic Compounds (18 Hrs)

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

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

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

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 Akampptisomerism(basic idea only)

4.2 Center of chirality: Molecules with C, N, S based chiral centers,absolute configuration, enantiomers, racemic modifications, R and S nomenclature using

Cahn-Ingold-Prelog rules,molecules with a chiral center and Cn, molecules with more than one center of chirality,definition of diastereoisomers, constitutionally symmetrical and unsymmetrical chiral molecules, erythro and threo nomenclature.

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

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

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

Unit 5: Conformational Analysis (18 Hrs)

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

5.2 Conformation and reactivity of elimination (dehalogenation, dehydrohalogenation, semipinacolic deamination and pyrolytic elimination - Saytzeff and Hofmann eliminations),substitution and oxidation of 2^0 alcohols.

5.3 Chemical consequence of conformational equilibrium - Curtin Hammett principle.

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2. F.A. Carey, R.A. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5thEdn., Springer, 2007.
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12. Jerry March, Advanced Organic Chemistry: Reactions, Mechanisms, and Structure
13. Nature Chemistry, Vol 10, 2018, pp 618 – 624.

CH 50 01 03 QUANTUM CHEMISTRY AND GROUP THEORY

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

Objective of the course

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

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

1.1. Symmetry elements and symmetry operations.

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

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

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

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

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

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

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

Unit 2 : Quantum Mechanics and Applications (36Hrs)

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

2.2. Postulates of Quantum Mechanics: State function or wave function postulate: Born interpretation of the wave function, well behaved functions, orthonormality of wave

functions. Operator postulate: Operator algebra, linear and nonlinear operators, Laplacian operator, commuting and noncommuting operators, Hermitian operators and their properties, eigen functions and eigen values of an operator.Eigen value postulate: eigen value equation, eigen functions of commuting operators.Expectation value postulate. Postulate of time-dependent Schrödinger equation, conservative systems and time-independent Schrödinger equation.

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

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

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

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

2.7. Quantum Mechanics of Hydrogen-like Atoms: Potential energy of hydrogen-like systems. The wave equation in spherical polar coordinates: separation of variables-r, theta and phi equations and their solutions, wave functions and energies of hydrogen-like atoms. Orbitals: Radial functions, radial distribution functions, angular functions and their plots. Dirac's relativistic equation for hydrogen atom (Elementary idea only).

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

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CH 50 01 04 THERMODYNAMICS, KINETIC THEORY AND STATISTICAL THERMODYNAMICS

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-Tiemannreaction. Reactions of ylides by carbenoid decomposition

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

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

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

Unit 5: Radical Reactions (9 Hrs)

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

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

Unit 6: Chemistry of Carbonyl Compounds (9 Hrs)

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

Unit 7: Concerted Reactions (18 Hrs)

7.1 Classification :Electrocyclic, sigmatropic, cycloaddition, chelotropic,ene and dyotropic reactions. Woodward Hoffmann rules - Frontier orbital and orbital symmetry correlation approaches - PMO method (for electrocyclic and cycloaddition reactions only).

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

7.3 Unimolecular pyrolytic elimnination reactions: Cheletropic elimination, decomposition of cyclic azo compounds, β-eliminations involving cyclic transition states such as N-oxides (Cope reaction), Acetates and Xanthates (Chugaeve reaction).

7.4 Problems based on the above topics

References

1. R. Bruckner, Advanced Organic Chemistry: Reaction Mechanism, Academic Press, 2002.
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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 of helium atom.

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

2.3 Hartree-Fock method,multi-electron atoms. Hartree-Fock equations (no derivation). The Fock operator, core hamiltonian, coulomb operator and exchange operator.Qualitative treatment of Hartree-Fock Self-Consistent Field (HFSCF) method. Roothan's concept of basis functions, Slater type orbitals (STO) and Gaussian type orbitals (GTO), sketches of STO and GTO.

Unit 3: Chemical Bonding (18 Hrs)

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

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

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

Unit 4: Computational Quantum Chemistry (18 Hrs)

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

4.2 Ab initio methods: A review of Hartee-Fock method,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.

References

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20. C.J. Cramer, Essentials of Computational Chemistry: Theories and Models, 2nd Edn., John Wiley & Sons, 2004.
21. D.C. Young, Computational Chemistry: A Practical Guide for Applying Techniques to RealWorld Problems, John Wiley & Sons, 2001.

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 04MOLECULAR 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, 4th Edn., Tata McGraw Hill, 1994.
2. G. Aruldhas, Molecular Structure and Spectroscopy, Prentice Hall of India, 2001.
3. A.U. Rahman, M.I. Choudhary, Solving Problems with NMR Specroscopy, Academic Press, 1996.
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SEMESTERS 1 AND 2

CH 50 02 05 INORGANIC CHEMISTRY PRACTICAL-1

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

Objective of the Course

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

PART I

Separation and identification of a mixture of four cations (a mixture of two familiar ions such as Ag^{+} , Hg^{2+}, Pb^{2+}, Cu^{2+}, Bi^{2+}, Cd^{2+}, As^{3+}, $Sn^{2+,}$ Sb^{3+}, Fe^{2+}, Fe^{3+}, Al^{3+}, Cr^{3+}, Zn^{2+} , Mn^{2+}, Co2+, Ni^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}, Mg^{2+}, Li^{+} , Na^{+} , K^{+} and $NH4^{+}$ and two less familiar metal ions such as Tl, W, Se, Mo, Ce, Th, Ti, Zr, V, U and Li). Anions which need elimination not to be given.Minimum eight mixtures to be given.

PART II

Colorimetric estimation of Fe, Cu, Ni, Mn, Cr, NH4+, nitrate and phosphate ions.

PART III

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

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

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

(c) Hexammine cobalt (III) chloride.

(d) Tetrammine copper (II) sulphate.

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

(f) Bis(dimethylglyoximato)nickel(II)

(g) Prussian blue

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

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

Objective of the Course

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

PART I

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

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

PART II

1. Separation of Organic binary mixtures by chemical/solvent separation methods
2. Quantitative separation of organic mixtures by column chromatography – Purity assessment of the components by TLC.

PART III

Drawing the reaction schemes (Based on Semester 1 and 2 theory) by ChemDraw, Symyx Draw and Chemsketch. Draw the structures and generate the IR and NMR spectra of the substrates and products in the following reactions:

1. Condensation
    (a) Dieckmann condensation
    (b) Claisen condensation
    (c) Darzen condensation
    (d) Aldol condensation

2. Oxidation / Reduction

   (a) Ozonolysis

   (b) Baeyer Villiger oxidation

   (c) Cannizaro reaction

   (d) Clemmenson reduction

3. Rearrangement

   (a) Benzilic acid rearrangement

   (b) Pinacol – Pinacolone rearrangement

   (c) Dienone – Phenol rearrangement

   (d) Wagner – Meerwein rearrangement

4. Pericyclic reaction

   (a) Diels – Alder reaction

   (b) Cope rearrangement

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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.

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SEMESTER 3

CH 04 03 01 SYNTHETIC AND BIOORGANIC CHEMISTRY

Credit:4 **Total Contact hours:72**

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 green chemistry and supramolecular chemistry

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

1.1 Survey of organic reactions with special reference to oxidation and reduction. Metal based and non-metal based oxidations of (a) alcohols to carbonyls [(Chromium-John's oxidation,Collin's oxidation, Sarrett oxidation),Manganese, aluminium and DMSO(Swernoxidation, Moffatt –Pfitzneroxidation, Kornblumoxidation, Corey-Kim oxidation)] based reagents (b) alkenes to epoxides (peroxides/per acids based)-Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation (c) alkenes to diols (Manganese and Osmium based)-Prevost reaction and Woodward modification (d) alkenes to carbonyls with bond cleavage (Manganese based, ozonolysis) (e) alkenes to alcohols/carbonyls without bond cleavage-hydroboration-oxidation, Wacker oxidation, selenium based allylic oxidation (f) ketones to ester/lactones- Baeyer-Villiger oxidation.

1.2 (a)Catalytic hydrogenation (Heterogeneous:Palladium/Platinum/Rhodium and Nickel. Homogeneous: Wilkinson). (b) Metal based reductions- Birch reduction, pinacol formation, acyloin formation (c)Enzymatic reduction using Baker's yeast.

Unit 2: Modern Synthetic Methods (9Hrs)

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

2.2 Multicomponent reactions:Ugireaction, Passerini reaction and Biginelli reaction.

Unit 3: Synthetic Reagents (9Hrs)

3.1. Hydride transfer reagents from Group III and Group IV in reductions - $LiAlH_4$, DIBAL-H, Red-Al, $NaBH_4$ and $NaCNBH_3$, selectrides, trialkylsilanes and trialkyl stannane. Aluminum isopropoxide (oxidation and reduction).Reagents such as NBS, DDQ and DCC.Gilmann reagent.DMAP-Borane, PCC,DEAD (Mitsunobu reaction).

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

4.1 Synthesis of four, five and six-membered rings- Photochemical approaches for the synthesis of four membered rings-oxetanes and cyclobutanes, ketene cycloaddition (inter and intra molecular), Pauson-Khand reaction, Volhardt reaction, Bergman cyclization, Nazarovcyclization,cation-olefin cyclization and radical-olefin cyclization.

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

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

5.1 Introduction to Supramolecular Chemistry, Host, Guest, host-guest complex formation, Lock and Key Principle, Pre-organistion, Complementarity

5.2 Concept of molecular recognition, Forces involved in molecular recognition.

5.3 Cation-binding hosts: Crown ethers, Cryptands, Spherand, calixarenes

5.4 Anion binding host- cyclophane

5.5 A naturally occurring cyclic host: Cyclodextrin- Industrial applications

Unit 6: Green Alternatives to Organic Synthesis (9 Hrs)

6.1 Principles of Green Chemistry: basic concepts, atom economy, twelve principlesof Green Chemistry, principles of green organic synthesis.

6.2 Green alternatives to Organic Synthesis: coenzyme catalysed reactions, thiamine catalyzed benzoin condensation. Green alternatives of molecular rearrangements: pinacol-pinacolone and benzidine rearrangements. Electrophilic aromatic substitution reactions.Oxidation-reduction reactions. Clay catalysed synthesis. Condensation reactions.Green photochemical reactions.

6.3 Green Solvents: ionic liquids, supercritical CO_2, fluorous chemistry.

6.4 General principles of microwave and ultrasound assisted organic synthesis.

Unit 7: Chemistry of Natural Products (9Hrs)

7.1 Alkaloids: Introduction, classification and biological activity of alkaloids. General methods of structural determination of alkaloids, structure elucidation of Morphine.

7.2 Flavonoids: Introduction, isolation and purification of flavonoids. General methods of structural determination of flavonoids.

7.3 Steroids: Introduction, nomenclature and structural elucidation of cholesterol.

7.4 Semisynthetic drugs derived from natural sources such as: Antibiotics (Erythromycin, new generation Cephalosporins) and Curcumin. Transformation of phytosterolsinto steroidal drugs

7.5 Marine natural products: Introduction and compounds of medicinal importance derived from marine sources such as Cytarabine and Ziconotide.

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   Press, 2001.
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CH 04 03 02 PHYSICAL CHEMISTRY

Credit: 4 **Contact Lecture 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, ,different thermodynamic parameters and photochemical reactions

Unit 1: Chemical Kinetics (18 Hrs)

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

1.2. Steady state approximation-chain reactions H_2-Br_2 Reaction, H_2-Cl_2 reaction

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

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

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

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

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

Unit 2: Surface Chemistry and Colloids (18 Hrs)

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

2.2 Application of low energy electron diffraction and photoelectron spectroscopy, ESCA and Auger electron spectroscopy, scanning probe microscopy, ion scattering, SEM and TEM in the study of surfaces.

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

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

Unit 3: Advanced Thermodynamics (9Hrs)

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

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

Unit4 : Photochemistry (9Hrs)

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

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

4.3 Quenching of fluorescence and its kinetics, Stern-Volmer equation, concentration quenching, fluorescence and structure, delayed fluorescence, E-type and P-type, effect of temperature on emissions, photochemistry of environment, greenhouse effect, application of pulsed laser in measuring the dynamics of photochemical processes. Photochemistry of vision.

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

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

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

5.5 Differential Thermal analysis(DTA); Principle, Instrumentation Advatages and disadvantages, Pharmaceutical applications, Derivative differential thermal analysis(DDTA), TGA: Principle, instrumentation, factors affecting results, advantages and disadvantages, pharmaceutical applications

Unit6: Diffraction Methods and Atomic Spectroscopic Techniques (9 Hrs)

6.1 Electron diffraction of gases. Wierl's equation. Neutron diffraction method. Comparison of X-ray, electron and neutron diffraction methods.

6.2 Atomic absorption spectroscopy (AAS), principle of AAS, absorption of radiant energy by atoms, classification of atomic spectroscopic methods, measurement of atomic absorption, instrumentation.

6.3 Atomic emission spectroscopy (AES), advantages and disadvantages of AES, origin of spectra, principle and instrumentation.

6.4 Flame emission spectroscopy (FES), flames and flame temperature, spectra of metals in flame, instrumentation and applications.

References

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CH 04 03 03DRUG DESIGN AND PHARMACOLOGY

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

Objective of the course

The learners should understand the principles of drug design and drug therapy, pharmacology,drugs and analgesics and its mode of action

Unit 1: Principles of Drug Therapy and Drug Design (27Hrs)

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

1.2 Drug action-receptor theories. Drug metabolism–different pathways.

1.3 Drug design: various factors of drug design, rational drug design. Methods of leaddiscovery: optimisation of the lead, natural and synthetic sources of leadcompounds. Bio isosterism. Prodrug and soft drug concept. Drug synthesis. Combinatorial synthesis (basic concepts).Retrosynthetic analysis of benzocaine, saccharin, salbutamol and benzodiazepines.

1.4 Basic concepts of CADD, Molecular Modeling: Energy minimization, geometry optimization, conformational analysis, globalconformational minima determination; Approaches and problems; Bioactive vs. global minimumconformations; Automated methods of conformational search; Advantages and limitations of availablesoftware; Molecular graphics; Computer methodologies behind molecular modeling including artificial intelligence methods

1.5 Molecular docking and dynamics: Rigid docking, flexible docking, manual docking; Advantages anddisadvantages of flex-X, flex-S, auto dock and dock softwares with successful examples; Monte Carlosimulations and molecular dynamics in performing conformational search, docking etc.

1.6 QSAR: Electronic effects; Lipophilicity effects; Hansch equation, Steric Effects; TaftEquation; Experimental and theoretical approaches for the determination of physico-chemical parameters, parameter inter-dependence; Case studies; Regression analysis, extrapolation versusinterpolation, linearity versus non-linearity; The importance of biological data in the correct form; 2D –QSAR; 3D-QSAR-examples CoMFA and CoMSIA.QSAR.

Unit 2: Pharmacology (9 Hrs)

2.1 General principles of pharmacology: biological response to drugs, passage of drugs across membranes.

2.2 Pharmacokinetic principles: absorption, distribution, metabolism and excretion of drugs. Dose of drugs and routes of administration.

2.3 Pharmacodynamic principles: dose response relationships, mechanism of drug action, unusual and adverse responses of drugs, structurally specific and nonspecific drugs. Ferguson's principle.

2.4 Drug interactions-synergism, antagonism, drug addiction and drug dependence, drug tolerance, drug hypersensitivity.

Unit 3: Inorganic Medicinal Chemistry (9 Hrs)

3.1 Gold Compounds for the Treatment of Rheumatoid Arthritis. Vanadium Salts as Insulin Mimics. Chelation Therapy- Metal Sequestration, Macrocyclic Antibiotics Metal Intoxication, Thalassaemia–Iron, Wilson Disease–Copper. Metal Complexes in cancer therapy.

3.2 Diagnostic Medicine: Magnetic Resonance Imaging Contrast Agents, X-ray Contrast Agents, Radiopharmaceuticals for Functional Imaging, Blood-pool Imaging and LabelledBlood Cells, Kidney Imaging.

Unit 4: Drugs acting on CNS (18 Hrs)

4.1 General anaesthetics. Inhalation anaesthetics - ether, enflurane, halothane, nitrousoxide, cyclopropane. Intravenous anaesthetics - thiopentone sodium, ketamine.

4.2 Hypnotics, sedatives and anxiolytic agents.

4.3 Anxiolytic agents-benzodiazepines, buspirone and meprobamate.

4.4 Anticonvulsants: convulsions, types of epilepsy, barbiturates-hydantoins, oxazolidinediones, succinimides and benzodiazepines.

4.5 Analeptics: xanthines, amphetamines, nikethamide and ethamivan.

4.6 Centrally acting muscle relaxants: glyceryl ethers-mephenesin, alkane diolderivatives-meprobamate, benzodiazepines-librium, diazepam and baclofen.

4.7 Antiparkinson's agents: dopamine agonists, dopamine releasing agents andsynthetic anticholinergics.

4.8 Drugs for Alzheimer's disease: cholinergic agonists and acetylcholine esteraseinhibitors.

4.9 Synthesis of the following drugs - Enflurane, Ketamine,Etomidate, Phenobarbital, Diazepam, Chlordiazepoxide, Meprobamate, Buspirone, Ethinamide, Nikethamide,

Ethamivan, Trimethadione, Ethosuximide, Denzimol, Topiramate, Mephenesin, Levodopa, Besiperidine and Tacrine.

Unit 5: Analgesics **(9 Hrs)**

5.1 Narcotic analgesics - morphine and its analogues, phenyl(ethyl) piperidines, diphenylheptanones and benzocaine derivatives.

5.2 Antipyretics and NSAIDs: Basic idea of COX I &I I inhibitors, salicylatesaspirin, p-aminophenol derivatives-paracetamol, phenacetin, pyrazolidinedionesphenylbutazone, oxyphenbutazone, anthranilicacid derivatives-mefanamic acid, flufenamicacid, indoleacetic acid derivatives-indomethacin, arylacetic/ propionicacid derivatives (ibuprofen, ketoprofen, flubiprofen and diclofenac), oxicams (piroxicam and tenoxicam).

5.3 Drugs used for gout - allopurinol, selective COX II inhibitors

5.4 Synthesis of the following drugs-levorphanol, pethidine, methadone, phenylbutazone, flufenamic acid, diclofenac, piroxicam, allopurinol and celicoxib.

References

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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,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

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SEMESTER 4

ELECTIVE COURSES

GROUP A

CH 86 04 01 BACTERIOLOGY AND BIOCHEMISTRY

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

Unit 1: Introduction to Microbiology (18Hrs)

1.1 Microorganisms and their role in diseases. A general study of viruses, fungi and protozoa. Properties of Viruses. Morphology of Viruses. Structure and Chemical Composition of the Viruses. Susceptibility to Physical and Chemical Agents. Viral Replication. Cultivation of Viruses. Detection of Virus Growth in Cell Culture. Viral Assay, Viral Genetics.

1.2 Morphology, classification and scientific nomenclature of bacteria. Growth requirements of bacteria and nutrientmedia. Staining of bacteria, theories of staining. Bacterial culture methods. Identification of bacteria. Bacterial genetics. General principles of microbialcontrol- sterilization and disinfection.

1.3 Bacteriology of water, milk and air.

1.4 Clinical Microbiology: Collection, handling and transport of specimens. Identification of microorganisms from specimens. Analysis of metabolic products.

Unit 2: Immunity (9 Hrs)

2.1 Types of immunity. Antigens and antibodies: theories of antigen-antibodyreactions, applications of antigen-antibody reactions. Structures and functions of the immune system.Interferons. Vaccines andsera - general study of the preparation of different types of vaccines, sera andtoxoids. AIDS.

Unit 3: Amino acids, Proteins and Nucleic Acids (18 Hrs)

3.1 Cells-classification and cell division.

3.2 Essential amino acids. Primary structure of proteins and amino acid analysis. Ramachandran plot and secondary structure of proteins. Tertiary structure andstructural motifs-protein folding and domain structure of proteins. Quaternarystructure of proteins. Purification and characterization of proteins. Functions of proteins. Chemical synthesis of proteins-protecting groups, solid phase peptidesynthesis.

3.3 DNA and RNA. Double helical structure of DNA. Replication of DNA.RNA. Classification of RNA.Genetic code. Nucleic acids as carriers of genetic information. Protein biosynthesis.DNA fingerprinting technique. Elementary principles of Recombinant DNA technology, gene therapy, cloning and bioinformatics.

Unit 4: Enzymes and Hormones(14Hrs)

4.1 Nomenclature and classification of enzymes. Mechanism of enzyme action. Substrate specificity of enzymes.Enzyme inhibition. Isoenzymes. Allosteric enzymes. Enzyme synthesis.Enzymes and digestion of food. Clinical uses of enzymes. Immobilization of enzymes. Clinical tests for sugar and cholesterol. ELIZA.

4.2 Functions and modes of actions of hormones. Pituitary, thyroid, parathyroid, pancreatic, adrenal and adrenocortical hormones. Antihormones.

Unit 5: Biological Oxidation and Metabolism (22Hrs)

5.1 ATP and ADP. Oxidative phosphorylation. Cytochromes.

5.2 Food as a source of energy. Calorific value of food. Basal metabolism. Respiratory quotient.

5.3 Carbohydrate metabolism: Glycogenesis and Glycolysis. Blood sugar level. Coricycle. The role of insulin. The citric acid cycle.Genetic and metabolic disorders. Diabetes mellitus (type 1 and type 2). Lipaemia.

5.4 Lipid metabolism. Essential fatty acids. Oxidation of fatty acids. Ketogenesis and ketosis.

5.5 Metabolism of amino acids and proteins. Oxidative deamination and trans- amination reactions. Urea formation-ornithine cycle. Inborn errors of metabolism.

Unit 6: Blood Composition and Acid Base Balance (9 Hrs)

6.1 Blood groups-Rh factor. Blood transfusion.Composition of blood cells. Chemistry of haemoglobin. Anaemias.Plasma proteins. Blood clotting- factors and mechanism. Coagulants.

6.2 Regulation of acid base balance. Acidosis and alkalosis.Renal function, formation and composition of urine.

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CH 86 04 02 ADVANCED PHARMACEUTICAL OPERATIONS AND DISPENSING

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

Unit 1: Pharmacognosy (27 Hrs)

1.1 Pharmacognosy of the official drugs frequently used in pharmacy: their sourcesand constituents. Eg:- senna, belladona, digitalis, stramonium,vasaka, cinnamon,cinchona, cannabis, ipecacuanha, rauwolfia, liquorice, ginger, cloves,pyrethrum, santonica, nutmeg, nuxvomica, cardamom, umbelliferous fruits like Cumin, Fennel, Caraway, Opium, Aloes, Asafoetida, Vincarosea, Brammi (two varieties).

1.2 Fixed oils and essential oil used in pharmacy-their sources. Extraction, constituents, composition analysis of fixed oils. : Castor oil, Olive oil, Shark liver oil. Essential Oils: Eucalyptus oil, Turpentine oil.

1.3 A brief study of the substances used as pharmaceutical necessities – Starches,Gum Acacia, Gum Tragacanth, Agar Agar, Gelatin, Talc, Kaolin. Bentonite.

Unit 2: Dispensing (9 Hrs)

2.1 Principles of dispensing medicaments. Incompatibilities and its overcoming.Preparation of pills, tablets, capsules, injectables, suppositories, coating of tablets.Newer Drug Delivery systems-site specific drug delivery systems in cancer chemotherapy to brain and CNS, to kidney and urinary tract. Implanted mechanical pumps.

Unit 3: Forensic Pharmacy (18 Hrs)

3.1 Pharmaceutical Legislation in India. Legal aspects of trade in drugs. The drug Actand Drug rules. The Pharmacy Act.The dangerous Drug Act and Rules. TheDrugs and Cosmetic Act and rules- Important definitions, Drugs Technical Advisory Board, Drugs Consultative Committee, Central Drugs Laboratory, The Schedules to the Act, Licensing and Controlling authorities and Rules regarding import, manufacture, storage, packing and labelling and sale of drugs and cosmetics.

3.2 Introduction to Pharmacopeia B.P, I.P. and general standard analysis.

3.3 Intellectual Property Rights (IPR), Patents, Patenting of pharmaceuticals, Indian Patent Act.

Unit 4: Pharmaceutical Analysis (18 Hrs)

4.1 Titrimetric Methods in Pharmaceutical Methods: Non-aqueous titrations, argentometric titrations, complexometric titrations, redox titrations, iodometric titrations, ion-pair titrations, diazotisation titrations and Karl Fischer titrations.

4.2 Applications of AAS, UV-Vis spectroscopy, IR-spectroscopy, NMR spectroscopy, Mass Spectrometry, TLC, GC and HPLC in pharmaceutical Analysis (theory and instrumentation not expected). Capillary Electrophoresis-Instrumentation and applications in pharmaceutical analysis.

4.3 Extraction Methods in pharmaceutical Analysis: Solvent Extraction methods and Solid phase Extraction.

Unit 5: Diagnostic Agents and Tests (18 Hrs)

5.1 Radiopharmaceuticals:Iodine radio nuclides, Technetium Radiopharmaceuticals, Nuclear medicine. RIA

5.2 Dyes used in pharmacy: Fluorescein, mercurochrome, acridine dyes.

5.3 Liver function tests :Prothrombine time, Hippuric acid test, serum albumin, serum globulin, ALP, AST, and Liver function alteration during diseases.

5.4 Gastric function tests: Measuring Gastric Acid in Basal and MaximalSecretory Tests.

5.5 Kidney function tests: BUN, Serum Creatine

5.6 Diagnosis of Heart diseases :Laboratory Diagnosis of Myocardial Infarction, Markers of Inflammation and CoagulationDisorders, Markers of Congestive Heart Failure, Patient-Focused Cardiac Tests . Tests for thyroid evaluation.

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CH 86 04 03 MEDICINAL CHEMISTRY

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

Unit 1: Drugs acting on ANS (18 Hrs)

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

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

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

1.4 Cholinergic blockers: tertiary and quaternary antimuscarinics, antispasmodicdrugs-dicyclomine, glycopyrrolate, antiulcer drugs-pirenzepine, cycloplegicdrugs-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 andprocainamide, β-blockers-propranolol. Calcium channel blockers-verapamil andNeurone blockers-bretilium.

2.3 Antihypertensive Drugs: peripheral antiadrenergics-prazosin and terazosin. Centrally acting drugs-reserpine, clonidine and methyl dopa. β-blockerspropranolol, atenolol and labetalol. Calcium channel blockers-nifedipine andamlodipine. 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-dipyridamoland aspirin.

2.5 Anticoagulants: heparin, coumarin derivatives and indanedione derivatives.

2.6 Antilipidemic agents: atherosclerosis(mention only), Statins-lovastatin, simvastatin, fluvastatin, Fibrates-clofibrate, Miscellaneous-bile acid sequestrantsand 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, abrief study of macrolide antibiotics, aminoglycoside antibiotics, polyeneantibiotics, fluoroquinolones.

3.2 Sulphonamides: sulphanilamide, N-substituted sulphanilamide derivatives,mechanism of action, sulphones-dapsone, dihydrofolatereductaseinhibitors, trimethoprimand cotrimoxazole.

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

3.4 Antifungal agents: Antibiotics-amphotericinB, griseofulvin and nystatin. Azolederivatives-ketoconozole,terconozole,fluconozole and clotrimazole.Pyrimidinederivatives- 5 Flucytosine.

3.5 Antiviral drugs: amantidine, interferon and ribavirin. Anti HIV agents zidovudine, and abacavir.Anti-herpes simplex agents-brivudine, vidarabin andacyclovir.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 andphenelzine. Tricyclic compounds-imipramine, trimipramine, amitriptynine, doxepine, amoxapine. Miscellaneous compounds-fluoxetine and trazodone.

5.3 Antipsychotics: phenothiazine and thiothixene derivatives, butyrophenoneshaloperidol, droperidon, rauwolfia alkaloids.

5.4 Hallucinogens: triptaminederivatives-DMT, psilocybin, phenylalkylaminesmescaline, 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 diureticsfurosemide and ethacrynic acid, potassium sparing diuretics-amiloride,spironolactone.

6.2 Antihistaminic drugs: histamine and its biological role, H1 antagonistsaminoalkylethers, 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, suphonylureastolbutamide, 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 syntheticsubstitutes-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 andranitidine, proton pump inhibitors-omeprazole and pantaprazole, digestants, carminatives and antidiarrheals.

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

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GROUP B

CH 87 04 01ADVANCED ORGANIC CHEMISTRY

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

Unit 1: Molecular Recognition and Supramolecular Chemistry (18 Hrs)

1.1 Introduction to supramolecular chemistry: Host, Guest, Host-Guest complex, Lock and key principle, Preorganisation, Complementarity.

1.2 Molecular recognition, forces involved in molecular recognition.

1.3 Cation binding Hosts: Crown ethers, Lariat ethers, Podands, Cryptands, Spherands, Calixarenes

1.4 Anion binding hosts: Cyclophanes. A naturally occurring cyclic host: Cyclodextrin - industrial applications.

1.5 Molecular clefts and tweezers. Macrocyclic polyamines – Nitrogen based cyclic hosts.

1.6 Naturally occurring Siderophores. Rhodopsin – A Supramolecular photonic device.

Unit 2: Green Alternatives to Organic Synthesis (9 Hrs)

2.1 Introduction to Green Chemistry: Atom economy

2.2 Twelve principles of Green Chemistry, How to plan a green synthesis.

2.3 Green Solvents: Ionic liquids, Supercritical CO2, Fluorous solvents, PEG

2.4 Microwave assisted organic synthesis – Principle, example.

2.5 Sonochemical synthesis – Principle, example

2.6 Green alternatives to organic synthesis: Thiamine catalyzed benzoin condensation, Montmorillonite K10 catalysed Pinacol-Pinacolone rearrangement, Photochemical reduction of benzophenone to benzopinacol, Synthesis of adipic acid from cyclohexene, Synthesis of Ibuprofen.

Unit 3: Biosynthesis and Biomimetic Synthesis (9 Hrs)

3.1 Basic principles of the biosynthesis of Terpenes, Steroids, Alkaloids, Carbohydrates, Proteins and Nucleic acids. Biosynthesis of Cholesterol, α- Terpineol, Morphine, Glucose and Phenyl alanine.Biogenesis of isoprenoids and alkaloids.Biomimetic synthesis of progesterone (Johnson synthesis).

Unit 4: Stereoselective Transformations (9 Hrs)

4.1 Assymmetric induction - Chiral auxiliaries and chiral pool.

4.2 Enantioselective catalytic hydrogenation developed by Noyori and Knowels.

4.3 Assymetricaldol condensation pioneered by Evans.

4.4 Assymmetric Diels-Alder reactions.

4.5 Enatioseletive synthesis of Corey lactone

Unit 5: Chemistry of Natural Products and Biomolecules (18 Hrs)

5.1 Synthesis of Camphor, Atropine, Papaverine, Quinine, Cyanin, Quercetin, β-Carotene, Testosterone, biosynthesis of PGE2 and PGF2α.

5.2 Structure of proteins, nucleic acids and methods for primary structure determination of peptides (N-terminal - Sanger's method and Edmond's method; C-terminal - Akabora method and carboxy peptidase method). Replication of DNA, Flow of genetic information, Protein biosynthesis, Transcription and translation, Genetic code, Regulation of gene expression, DNA sequencing.The Human Genome Project.DNA profiling and the Polymerase Chain Reaction (PCR).

Unit 6: Medicinal Chemistry and Drug Designing (9 Hrs)

6.1 Introduction to Drug design: Modeling techniques, Receptor proteins, Drug-receptor interaction, Drug action, Drug selectivity, Drug metabolism (Phase I and Phase II).

6.2 Mode of action of Warfarin (anticoagulant), Organic nitrates (anti-anginal drug), Captoril (antihypertensive agent), Chloroquin (antimalarial drug).

6.3 Antibiotics: Penicillins (SAR expected). Mode of action of chloramphenicol, Tetracyclins and Cephalosporins.Drugs for cancer (Methotrexate), AIDS (Zidovudin) and diabetes (Metformin).

Unit7: Advances in Polymer Chemistry (9 Hrs)

7.1 Conducting polymers, temperature resistant and flame retardant polymers, polymers for medical applications.

7.2 Dendrimers and dendritic polymers: Terminology, Classification of dendrimers. Methods of synthesis: convergent and divergent approaches. Applications of dendrimers. Hyperbranched polymers: definition, synthesis, applications.

Unit 8: Research Methodology of Chemistry (9 Hrs)

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

8.2 Types of research: Fundamental, applied, historical and experimental research.

8.3 Chemical literature: Primary, secondary and tertiary sources of literature. Classical and comprehensive reference. Literature databases: ScienceDirect, SciFinder. Chemical abstract.

8.4 Scientific writing: Research reports, thesis, journal articles, books. Types of publications: articles, communications, reviews.

8.5 Important scientific and Chemistry Journals. Impact factor.

References

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CH 87 04 02 ADVANCED PHARMACEUTICAL OPERATIONS AND DISPENSING

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

Unit 1: Pharmacognosy (27 Hrs)

1.1 Pharmacognosy of the official drugs frequently used in pharmacy: their sources and constituents. Eg:- senna, belladona, digitalis, stramonium, vasaka, cinnamon, cinchona, cannabis, ipecacuanha, rauwolfia, liquorice, ginger, cloves,pyrethrum, santonica, nutmeg, nuxvomica, cardamom, umbelliferous fruits like Cumin, Fennel, Caraway, Opium, Aloes, Asafoetida, Vincarosea, Brammi (two varieties).

1.2 Fixed oils and essential oil used in pharmacy-their sources. Extraction, constituents, composition analysis of fixed oils. : Castor oil, Olive oil, Shark liver oil. Essential Oils: Eucalyptus oil, Turpentine oil.

1.3 A brief study of the substances used as pharmaceutical necessities – Starches, Gum Acacia, Gum Tragacanth, Agar Agar, Gelatin, Talc, Kaolin. Bentonite.

Unit 2: Dispensing (9 Hrs)

2.1 Principles of dispensing medicaments. Incompatibilities and its overcoming. Preparation of pills, tablets, capsules, injectables, suppositories, coating of tablets. Newer Drug Delivery systems-site specific drug delivery systems in cancer chemotherapy to brain and CNS, to kidney and urinary tract. Implanted mechanical pumps.

Unit 3: Forensic Pharmacy (18 Hrs)

3.1 Pharmaceutical Legislation in India. Legal aspects of trade in drugs. The drug Actand Drug rules. The Pharmacy Act.The dangerous Drug Act and Rules. The Drugs and Cosmetic Act and rules- Important definitions, Drugs Technical Advisory Board, Drugs Consultative Committee, Central Drugs Laboratory, The Schedules to the Act, Licensing and Controlling authorities and Rules regarding import, manufacture, storage, packing and labelling and sale of drugs and cosmetics.

3.2 Introduction to Pharmacopeia B.P, I.P. and general standard analysis.

3.3 Intellectual Property Rights (IPR), Patents, Patenting of pharmaceuticals, Indian Patent Act.

Unit 4: Pharmaceutical Analysis (18 Hrs)

4.1 Titrimetric Methods in Pharmaceutical Methods: Non-aqueous titrations, argentometric titrations, complexometric titrations, redox titrations, iodometric titrations, ion-pair titrations, diazotisation titrations and Karl Fischer titrations.

4.2 Applications of AAS, UV-Vis spectroscopy, IR-spectroscopy, NMR spectroscopy, Mass Spectrometry, TLC, GC and HPLC in pharmaceutical Analysis (theory and instrumentation not expected). Capillary Electrophoresis-Instrumentation and applications in pharmaceutical analysis.

4.3 Extraction Methods in pharmaceutical Analysis: Solvent Extraction methods and Solid phase Extraction.

Unit 5: Diagnostic Agents and Tests (18 Hrs)

5.1 Radiopharmaceuticals:Iodine radio nuclides, Technetium Radiopharmaceuticals, Nuclear medicine. RIA

5.2 Dyes used in pharmacy: Fluorescein, mercurochrome, acridine dyes.

5.3 Liver function tests : Prothrombine time, Hippuric acid test, serum albumin, serum globulin, ALP, AST, and Liver function alteration during diseases.

5.4 Gastric function tests: Measuring Gastric Acid in Basal and MaximalSecretory Tests.

5.5 Kidney function tests: BUN, Serum Creatine

5.6 Diagnosis of Heart diseases :Laboratory Diagnosis of Myocardial Infarction, Markers of Inflammation and Coagulation Disorders, Markers of Congestive Heart Failure, Patient-Focused Cardiac Tests . Tests for thyroid evaluation.

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CH 87 04 03 INDUSTRIAL OILS AND FAT PRODUCTS

Credit 4 **Lecture Hours : 90 Hrs**

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

1.1. Mechanical pre treatment and heat treatment of oil bearing materials. Rendering of 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: Oils and 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.

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

13. E. Guenther, The Essential Oils, Vol I-VI, Van Nostrand, 1972.

14. L.H. Meyer, Food Chemistry, Reinhold, 1960.

SEMESTERS 3 and 4

CH 04 04 05 PHARMACEUTICAL ANALYSIS PRACTICAL

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

I. Preparation and limit test prescribed in IP/BP of the following drugs

(a) Sodium Salicylate (b) Calcium Lactate

(c) Ferrous Fumarate (d) Light Magnesium Carbonate

(e) Sodium Citrate

II. Assay and purity of following synthetic drugs and Vitamins

(a) Aspirin (b) Paracetamol (c) Isoniazide

(d) Ibuprofen (e) Riboflavin (f) Ascorbic acid

III. Colorimetric/Spectrophotometric Estimation of the following drugs

(a) Aspirin (b) Curcuminoids

(c) Paracetamol (d) Gingiberene

(e) Caffeine (f) Aceclofenac

IV. Simultaneous Estimations of

(a) Paracetamol & Ibuprofen

(b) Aspirin & Caffeine

(c) Aceclofenac &Paracetamol.

V. Assay of drugs by Potentiometric method of analysis.

(a) Cimetidine (b) Nitrazepam (c) Clonidine

References

1. A.O. Bentley, J.E. Driver, Bentley and Driver's Textbook of Pharmaceutical Chemistry, 7th Edn, Oxford University Press, 1960.
2. G.L. Genkins, A.M. Knevel, F.E. DiGangi, Quantitative Pharmaceutical Chemistry, 7th Edn, McGraw Hill, 1977.
3. K.A. Connors, A Textbook of Pharmaceutical Analysis, John Wiley & Sons, 2007.

4. Indian Ministry of Health and Family Welfare, Indian Pharmacopoeia 1996, Controller of Publication, 2000.

5. British Pharmacopoeia Commission, British Pharmacopoeia:2012 Edition, Bernan Assoc, 2011

CH 04 04 06 DRUG SYNTHESIS AND DISPENSING PRACTICAL

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

1. Synthesis of some typical organic medicinal compounds, spectral illustration of the intermediates and products formed: paracetamol, sulphanilamide, hippuran, benzocaine, clofibrate, mercurochrome, phenytoin, dapsone, diodoquin, antipyrine, aminacrine and phenobarbitone.

2. Preparation of some specified crude plant extracts and qualitative analysis (chemical or TLC) of crude plant extracts/ products to detect the presence of phytochemicals- alkaloids, carbohydrates, glycosides, tannins, flavanols and saponins.

3. **Isolation of phytochemicals from their natural sources.**

Examples

Caffeine from Tea

Nicotine from tobacco

Cucumin from turmeric

Tannins from Gallnuts

Lycopene from tomato

4. **Dispensing**

1. **Emulsions**

a. Castor oil emulsion

b. Shark liver oil emulsion

c. Liquid paraffin emulsion

2. **Liniments**

a. Turpentine liniment

b. Methyl salicylate liniment

c. Camphor liniment

3. **Ointments**

a. Compound benzoic acid ointment

b. Non-staining iodine ointment

4. **Pastes**

   a. Unnas paste

   b. Magnesium sulphate paste

5. **Creams**

   a. Vanishing cream

   b. Cetrimide cream

6. **Paints**

   a. Mandel's paint

   b. Tannic acid glycerine paint

7. **Lotions**

   Calamine lotion

8. **Dentrifices**

   a. Tooth paste

   b. Tooth powder

9. **Mixtures**

   Typical mixtures involving incompatibilities.

10. **Tablets**

    a. Aspirin tablet

    b. A P C tablets

References

1. T. E. Wallis, Practical Pharmacognosy, Churchill, 1948.
2. A.O. Bentley, J.E. Driver, Bentley and Driver's Textbook of Pharmaceutical Chemistry, 7thEdn., Oxford University Press, 1960.
3. K.A. Connors, A Textbook of Pharmaceutical Analysis, John Wiley & Sons, 2007.
4. J.W. Cooper, C. Gunn, Cooper and Gunn's Dispensing for Pharmaceutical Students, Pitman Medical, 1967.
5. A. Kar, Advanced Practical Medicinal Chemistry, New Age International, 2007.

CH 04 04 07BIOCHEMISTRY AND BACTERIOLOGY PRACTICAL

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

A. Biochemistry

1. Blood Analysis

a. Determination of blood group and Rh factor.

b. Enumeration of RBC, WBC and differential leucocyte count.

c. Determination of ESR.

d. Estimation of urea, uric acid, cholesterol, creatinine, haemoglobin and calcium.

2. Urine Analysis

a. Qualitative analysis of urine for the common pathological constituents-sugar, albumin, ketone bodies, bile.

b. Estimation of albumin, ketone bodies, sugar and urea.

3. Milk Analysis

Estimation of specific gravity, total solids, fat, lactose, total nitrogen, calculation of percentage of added water.

4. Water Analysis

Estimation of total dissolved matter, chloride, saline and albuminoid ammonia and COD.

5. Preparation of some compounds of biochemical interest.

Examples: caffeine, albumin, glutamic acid, urease, cholesterol, tyrosine.

6. Separation of amino acids by paper chromatography.

7. Separation of serum proteins by paper electrophoresis.

B. Bacteriology

1. **Preparation of some typical nutrient media for collection and isolation of bacteria.**

a. Nutrient Agar, Endo's Agar, Chapman's Agar, Tergotol-7 Agar and McConkey Agar.

2. **Staining and the study of the morphology of the bacteria.**

   a. Simple stain

   b. Gram stain (Huker method)

   c. Capsule stain

   d. Acid fast stain (Ziehl- Neelson)

   e. Negative stain (India ink method)

3. Fermentation test

4. Identification of some common pathogenic organisms.

5. Enumeration of bacteria in water.

6. Enumeration of bacteria in milk-the reductase test.

7. Evaluation of germicides-Riedel Walker test.

8. Antibiotic sensitivity tests.

9. Preparation and standardization of vaccines.

10. Preparation of lactic acid by fermentation of sugar.

11. Method of study of antibacterial activity of compounds and complexes.

References

1 A.J. Salle, Laboratory Manual of Fundamental Principles of Bacteriology, McGraw Hill, 1973.

2 R.C. Goss, Experimental Microbiology Laboratory Guide, Iowa State Univ. Press, 1967.

3 T.J. Mackie, J.E. McCartney, Handbook of Practical Bacteriology, E&S Livingstone, 1948.

4 P.B. Hawk, Hawk's Physiological Chemistry, Blakiston Division, 1965.

5 K. Wilson and J.M. Walker, Principles and Techniques of Practical Biochemistry, 5thEdn., Cambridge University Press, 2000.

6 M.B. Jacob, The Chemical Analysis of Food and Food products, Van Nostrand, 1958.

7 J.A. Kolmer, E.H. Spaulding, H.W. Robinson, Approved Laboratory Techniques, Appleton Century Crofts, 1951.

8 D.T. Pulmmer, An Introduction to Practical Biochemistry, McGraw Hill, 1987.

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MODEL QUESTION PAPERS

QP Code **Reg. No. …..**

Name ……

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

First Semester

Faculty of Science- Chemistry

CH04 Pharmaceutical 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

CH04 Pharmaceutical Chemistry

CH 50 01 02 STRUCTURAL AND MOLECULAR ORGANIC CHEMISTRY

(Common for all branches of Chemistry)

(2019 admissions onwards)

Time: Three hours Max. Weight: 30

Section- A

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

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

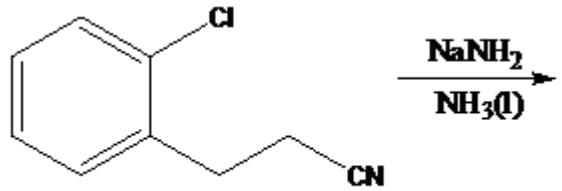
(8 x 1 = 8)

Section B

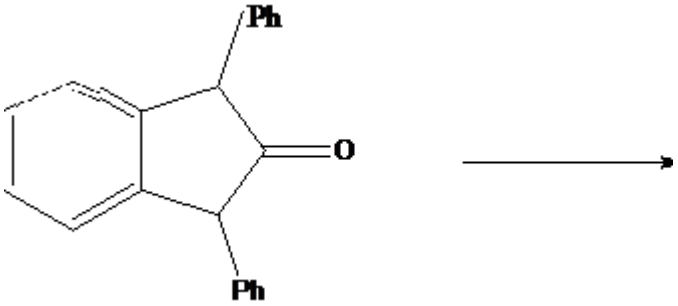
(Answer any **six** questions. Each question carries a weight of 2)

11. Predict the product and explain the mechanism

a)



b)



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

13. Write a note on Fullerenes and Graphene.

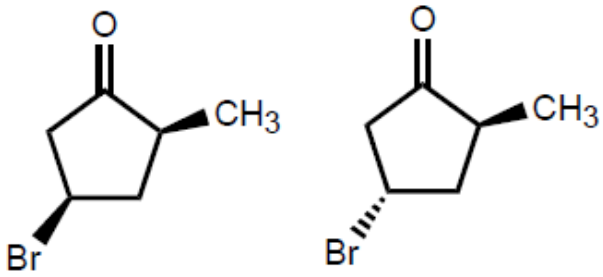
14. What are hard and soft acids? Use HSAB principle to distinguish them

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

16. Explain Curtin Hammett principle

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

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



(6 x 2 = 12)

Section C

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

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

b)Explain the mechanism of semipinacolic deamination.

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

21. Explain the Nucleophilic substitution reactions in aromatic systems

22. Explain in detail about;

a) Carbon based chiral centers.

b) N based chiral centers.

c) S based chiral centers.

(2 x 5 = 10)

QP Code **Reg. No. …..**

Name ……

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

First Semester

Faculty of Science- Chemistry

CH04 Pharmaceutical Chemistry

CH 50 01 03-Quantum Chemistry and Group Theory

(Common for all branches of Chemistry)

(2019 admissions onwards)

Time: Three hours **Max. Weight: 30**

Section- A

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

1. Predict the point group of (i) glyoxal (ii) cis-$[Co(en)_2Cl_2]^+$
2. Explain 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
CH04 Pharmaceutical 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 $4.59 \times 10^{-47} Kgm^2$ symmetry number $\sigma=2$.

(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 graphicalrepresentation.

21. (a) Derive an expression for Fermi-Dirac statistics (b) Give comparative account of the three statistics.

22. Derive Debye theory of heat capacity of solids. How does it differ from Einstein theory?

(2 x 5 = 10)

QP Code **Reg. No. …..**

Name ……

M.Sc Degree (C.S.S) Examination, ……

Second Semester

Faculty of Science- Chemistry

CH04 Pharmaceutical 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

CH04 Pharmaceutical Chemistry

CH500202- ORGANIC REACTION MECHANISM

(Common for all branches)

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

Second Semester

Faculty of Science- Chemistry

CH04 Pharmaceutical Chemistry

CH 50 02 03-Chemical Bonding and Computational Chemistry

(Common for all branches of Chemistry)

(2019 admissions onwards)

Time: Three hours Max. Weight: 30

Section- A

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

1. What are slater determinants?

2. State and Explain Variation theorem

3. State and explain Non crossing rule in quantum mechanics

4. Explain Hellmann-Feynmann theorem.

5. Find out the characters for all the symmetry operations of NH_3 molecule using Cartesian coordinates.

6. What are the group theoretical selection rules for an electronic transition to be allowed?

7. Explain AMBER.

8. What is CHARMM? Explain its use in molecular mechanics.

9. What is Koopman's Theorem?

10. Write a short note on Independent Electron Approximation **(8 x 1 = 8)**

Section B

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

11. Illustrate variation theorem using the trial wave function x(a-x) for particle in a one dimensional box

12. Explain Huckel molecular orbital theory of Butadiene and Benzene

13. Explain how group theory helps to predict optical activity

14. Using Direct Product Tables, predict the electronic transitions of C_2v and C_3v molecules.

15. What are the important assumptions used in HFSCF method ?

16. Explain how to build a Z-matrix?

17. Compare MOT and VBT

18.Explain the Kohn-Sham approach used in DFT? **(6 x 2 = 12)**

Section C

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

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

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

21. Explain Perturbation Method? Illustrate with Helium as Example

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

(2 x 5 =10)

QP Code **Reg. No. …..**

Name ……

M. Sc Degree (C.S.S) Examination, ……

Second Semester

Faculty of Science- Chemistry

CH04 Pharmaceutical Chemistry

CH 50 02 04–Molecular Spectroscopy

(Common for all branches of Chemistry)

(2019 admissions onwards)

Time: Three Hours Maximum Weight: 30

Section A

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

1.What is FID and FT in NMR spectroscopy?

2. What is Born Oppenheimer approximation? Explain the cases where the Born Oppenheimer approximation breaks down.

3. What is fermi resonance? Give one example.

4**.** Explain mutual exclusion principle**.**

5. Which of the following molecules exhibit pure rotational spectra? HF, NH_3 ,H_2O , CO, CH_4 , BF_3 , CO_2 , F_2 .

6. Differentiate between first order and second order NMR spectra

7. What are fine structure and hyperfine structure in ESR spectrum?

8. What is Resonance Raman Spectrum?

9. What is finger print region in IR?

10. Discuss Frank condon principle. **(8 × 1 =8)**

Section B

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

11. Explain the basic principle of NQR spectroscopy.

12. Give the applications of ESR and Mossbauer methods in spectroscopy

13. Explain the terms chemical shift, coupling constant and factors influencing coupling constant in NMR spectroscopy

14. The first line in the rotational spectrum of NO appears at 1.72 cm^{-1} and its force constant is 1608 Nm^{-1}. Calculate the internuclear distance in A^0, vibrational frequency in cm^{-1} and energy in joules required for J = 3 to 4 rotational transition.

15. The first three vibrational energy of HCl were found to be at 2886, 5668 and 10923 cm^{-1}. Calculate the anharmonicity constant, zero point energy and the equilibrium oscillation frequency. Calculate the centrifugal distoration constant if the rotational constant is 21.18 cm^{-1}16. Discuss photoelectron spectroscopy.

17. Explain the various relaxation methods in NMR.

18. What is meant by normal mode of vibration? How many normal modes of vibration do the following molecules have? NH_3 , HCN , SO_2

(6 × 2 = 12)

Section C

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

19. Explain the following in NMR spectroscopy

    a) Larmor Precision

    b) Chemical shift and its representation

    c) Magic angle spinning

20. Explain the classical theory of Raman spectroscopy.

21. Discuss the theory and applications of NQR Spectroscopy.

22. Write note on:

    a) Resonance fluorescence

    b) Predissociation

    c)Mechanism of Laser action

    d) Polarized and depolarized Raman lines **(5 × 2 = 10)**

QP Code **Reg. No. …..**

Name ……

M. Sc Degree (C.S.S) Examination, ……

Third Semester

Faculty of Science- Chemistry

CH04 Pharmaceutical Chemistry

CH 04 03 01 -Synthetic and Bioinorganic Chemistry

(2019 admissions onwards)

Time: Three hours Max. Weight: 30

Section- A

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

1. Sketch the mechanism of Sarrett oxidation.

2. What are the applications of Wacker oxidation?

3. What are the advantages of reduction using Baker's yeast?

4. Write the mechanism of Brook rearrangement

5. What do you mean by molecular recognition?

6. What are the important industrial applications of cyclodextrins?

7. Mention the advantages of thiamine catalyzed benzoin condensation.

8. Write an example for clay catalysed synthetic reaction.

9. Comment on the uses of Ziconotide.

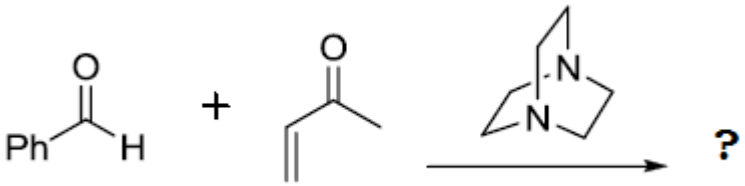
10. What is Gilmann reagent? What are its uses?

(8 x 1 = 8)

Section B

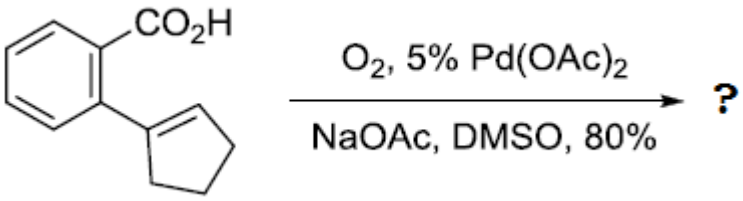
(Answer any **six** questions. Each question carries a weight of 2)

11. Complete the reaction and write the mechanism of the reaction.

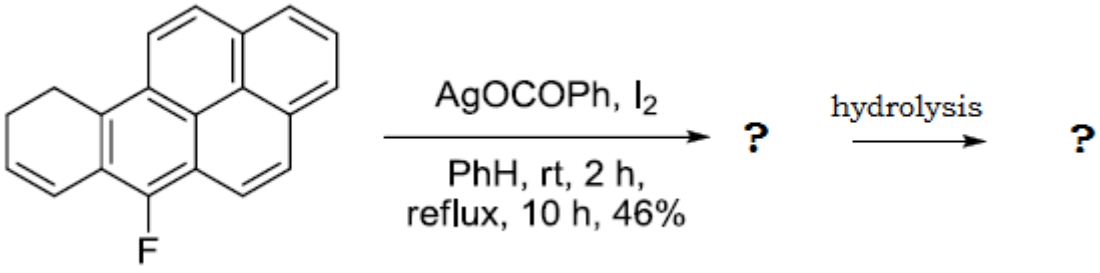


12. Give the structure of the products in the following reactions:

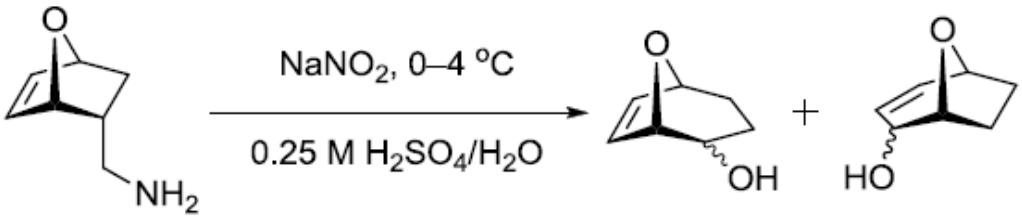
a)



b)

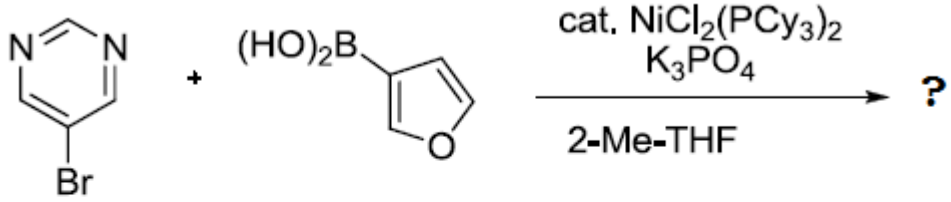


13. Write the mechanism of the following reaction



14. Complete the following reactions.

a)



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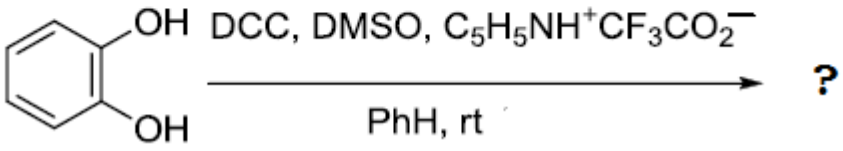


15. Write a note on cation binding hosts.

16. Give an account of green solvents.

17. Discuss classification and biological activity of alkaloids.

18. Write a note on the construction of macrocyclic rings. (**6 x 2 = 12**)

Section C

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

19. Discuss different methods for the epoxidation of alkenes. Write mechanism of each method and give their applications.

20. a) Write a note on the multicomponent reactions, Ugireaction, Passerini reaction and Biginelli reaction.

b) Explain uses of the reagents NBS, DDQ and DCC.

21. a) Discuss one method each for the synthesis of four, five and six membered rings.

b) Give an account of forces involved in molecular recognition with suitable examples.

c) Discuss the 12 principles of green chemistry.

22. Describe the structure elucidation of Morphine. (**2 x 5 = 10**)

QP Code **Reg. No. …..**

Name ……

M Sc Pharmaceutical Chemistry Chemistry Degree (C.S.S) Examination, ……

Third Semester

Faculty of Science- Chemistry

CH04 Pharmaceutical Chemistry

CH 04 03 02-PHYSICAL CHEMISTRY

(2019 admissions onwards)

Time: Three hours Max. Weight: 30

Section- A

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

1Give the significance of $\Delta S^{\neq}$.

2. What is Skrabal diagram?

3. Mention important applications of Surface Enhanced Raman Scattering?

4. What is zeta potential?

5. What is the principle of microscopic reversibility?

6. What is quantum yield?

7. Write down the advantages of coulometry.

8. Give an account of the pharmaceutical applications of DTA.

9. What are the disadvantages of AES?

10. List the important applications of ESCA. **(8 x 1 = 8)**

Section B

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

11. If a first-order reaction has an activation energy of 104600 J mol^{-1} and a pre-exponential factor A of 5 X 10^{13} s, at what temperature will the reaction have a half-life of (a) 1 min and (b) 30 days?

12. A solution absorbs 300 nm radiation at the rate of 1 W. What does this correspond to in amount of photons absorbed per second?

13. Discuss the kinetics of H_2-Br_2 Reaction.

14. Write a note on the use of SEM and TEM in the study of surfaces.

15. Derive Michelis-Menten equation.

16. Discuss the principle, instrumentation and applications of TGA.

17. Give an account of the principles and applications of FES.

18. Write a note on the photochemistry of vision. (**6 x 2 = 12**)

Section C

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

19. What are the factors determining reaction rates in solutions? Derive Bronsted-Bjerrum equation. Discuss primary and secondary kinetic salt effect

20. Outline Langmuir and BET theories of adsorption. Describe Use of Langmuir and BET isotherms for surface area determination.

21. a) What are coupled reactions? Discuss the role of ATP in bioenergetics.

    b) Give an account of thermodynamic aspects of metabolism and respiration and glycolysis.

22. a) Discuss the principle and applications of amperometric titrations.

    b) Write a note on the principle, instrumentation and applications of AAS. (**2 x 5 = 10)**

QP Code **Reg. No. …..**

Name ……

M Sc Pharmaceutical Chemistry Degree (C.S.S) Examination, ……

Third Semester

Faculty of Science- chemistry

CH04 Pharmaceutical Chemistry

CH 04 03 03-Drug Design and Pharmacology

(2019 admissions onwards)

Time: Three hours Max. Weight: 30

Section- A

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

1. 1What is molecular docking?
2. Explain how 3D structures are generated in 3D QSAR.
3. What is a pharmacophore?
4. Distinguish between agonist and antagonist.
5. What are orphan drugs?
6. Give a method of preparation of yellow mercuric oxide.
7. How do sedatives differ from hypnotics?
8. Discuss the importance of monooxygenases.
9. Name an analeptic and give its structure.
10. Give an example for a COX II inhibitor and draw its structure. **(8 x 1 = 8)**

Section B

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

11. Discuss modern receptor theories of drug action.
12. Give an account of the synthesis of i) diclofenac and ii) piroxicam
13. Explain the toxicity of lead in man.

14. What are anticonvulsant drugs? How are they classified? Explain with suitable examples.

15. Write a note on narcotic analgesics.

16. Discuss SAR of intravenous anaesthetics–thiopentone sodium and ketamine.

17. Discuss the importance of Hansch's analysis in drug design.

18. Write notes on COX I and COX II inhibitors. (**6 x 2 = 12**)

Section C

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

19. What is retrosynthetic analysis? Discuss retrosynthetic analysis of benzocaine, salbutamol and saccharin.

20. Explain the importance of physicochemical parameters and chemical structural aspects in determining the bioactivity of drug molecules.

21. Discuss the synthesis and medicinal applications of a) phenobarbital b) nikethamide c) flufenamic acid and d) celicoxib.

22. a) Discuss the preparation and medicinal applications of i) calcium gluconate, ii) magnesium stearate and iii) ferric ammonium citrate.

    b) Discuss the metabolism of drugs. What are important phase I metabolic reactions?

(**2 x 5 = 10**)

QP Code **Reg. No. …..**

Name ……

M.Sc Degree (C.S.S) Examination, ……

Third Semester

Faculty of Science- Chemistry

CH04 Pharmaceutical Chemistry

CH 50 03 04 – Spectroscopic Methods in Chemistry

(Common for all branches of Chemistry)

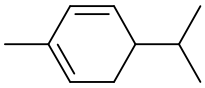
(2019 admissions onwards)

Time: Three hours **Max. Weight: 30**

Section- A

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

1. Calculate the λ_{max} for the compound



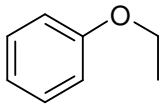
2. Which of the following isomers of pentadiene will show the largest wavelength of UV absorption? Give reason.

i) CH_2=CH-CH=CH-CH_3 ii) CH_2=CH-CH_2-CH=CH_2

3. 2-Hydroxy-3-nitroacetophenone shows two carbonyl stretching frequencies at 1692 and 1658 cm^{-1}. Explain.

4. C-H stretching frequency increases from alkane → alkene → alkyne. Explain.

5. Show the formation of the peak at m/z = 94 in the mass spectrum of



6. Predict the number of signals and sketch the NMR spectrum of CH_3-O-CH_2-CH_2-Cl.

7. What are shift reagents in NMR spectroscopy? Explain.

8. How NMR spectroscopy is useful in distinguishing cis-stilbene and trans-stilbene?

9. Explain off resonance decoupling.

10. Explain the spin notation A_2X_3 in NMR spectroscopy with example.

(8 × 1 =8)

Section B

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

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

12. Discuss the effect of concentration on vibrational stretching frequency of methyl salicylate and ethanol.

13. A compound with molecular formula $C_4H_8O_3$ gave the following spectral data. Deduce the structure. IR: 1120, 1705 cm^{-1} ^{1}H NMR: δ 12.1(1H, s), 4.15(2H, s), 3.6(2H, q, J = 7 Hz) and 1.3(3H, t, J = 7 Hz) ppm

14. Write a note on HRMS and MS-MS.

15. Explain McLafferty rearrangement.

16. Discuss the technique - spectral editing based on DEPT.

17. Briefly explain cross polarization and selective population inversion in NMR spectroscopy.

18. A compound 'A' with molecular formula C_5H_{10} on ozonolysis gives 'B', C_4H_8O, as one of the products. The IR spectrum of B showed a band at 1720 cm^{-1} and the NMR spectrum showed three signals at δ values 0.9 (3H, t), 3.4 (2H, q) and 2.2 (3H, s). What are A and B? Explain.

(6 × 2 = 12)

Section C

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

19. Describe the following

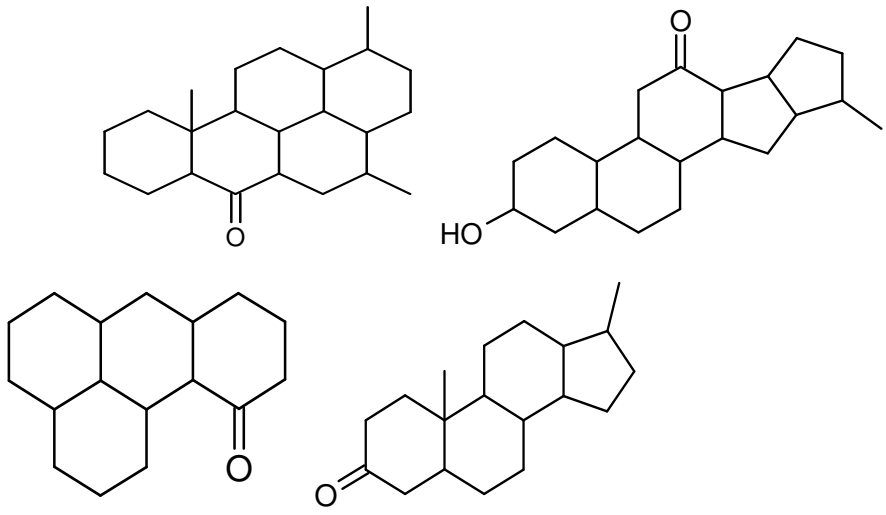
    a) FAB b) MALDI c) Field desorption d) TOF e) Cyclotron

20. Predict the structure of the compound (MF $C_{11}H_{20}O_4$) which gave the following spectral data. UV – No λ_{max} above 200 nm IR: 1740 cm^{-1}. ^{1}HNMR: δ 4.2 (4H, q), 3.3 (1H, t), 1.9 (2H, q), 1.33 (4H, m), 1.27 (6H, t) and 0.9 (3H, t) ppm. ^{13}C NMR: δ 14.10, 13.81, 22.4, 28.5, 29.5, 52.0, 61.1 and 169.3 ppm. Mass: m/z 216 ($M^{+\cdot}$), 171, 160 (100%), 133 and 115.

21. (a). Explain the magnetic anisotropy in carbonyl compounds and acetylene.

    (b). Define spin – spin coupling. Explain spin-spin coupling in the spin systems AX_2, AMX and ABC with examples.

22. Discuss Octant rule. Draw the octants for the following compounds and predict the sign of their optical activity.



(5 × 2 = 10)

QP Code **Reg. No. …..**

Name ……

M. Sc Pharmaceutical Chemistry Degree (C.S.S) Examination, ……

Fourth Semester

Faculty of Science- Chemistry

CH04 Pharmaceutical Chemistry

CH 86 04 01-Bacteriology and Biochemistry

(2019 admissions onwards)

Time: Three hours Max. Weight: 30

Section- A

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

1. 1. Which groups on amino acids react to form a peptide bond?
2. What are supersecondary structures (motifs) of proteins?
3. Explain why glycine and proline residues are not commonly found in helices.
4. What is feedback inhibition?
5. What is the effect of substrate concentration on enzyme action?
6. What are the common causes for hyperthyroidism?
7. Define oxidative phosphorylation.
8. Discuss the effect of ATP on gluconeogenesis.
9. Why is pyruvate not oxidized to CO_2, and H_2O under anaerobic conditions?
10. How does the redox potential of a conjugate redox pair is measured?

(8 x 1 = 8)

Section B

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

11. Discuss metabolic acidosis and respiratory acidosis.
12. How are enzymes classified? Explain with suitable examples.

13. Write a note on the quaternary structure of proteins. What are the advantages of quaternary associations?

14. Describe the structural differences between RNA and DNA.

15. What are the general functions of hormones in the body?

16. Describe the important roles of the citric acid cycle.

17. Discuss the structure of viruses.

18. Describe the functions of different classes of immunoglobulins.

(**6 x 2 = 12**)

Section C

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

19. (a) Discuss Enzyme inhibition.

    (b) Discuss the functions of thyroid and parathyroid hormones.

20. (a) Explain Cori cycle.

    (b) Write a note on the biosynthesis of fatty acids.

21. (a) Explain the mechanism of blood clotting

    (b) Write a note on buffer systems in blood.

22. (a) Describe nomenclature and structure of prostaglandins.

    (b) Discuss ornithine cycle (**2 x 5 = 10**)

QP Code **Reg. No. …..**

Name ……

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

Fourth Semester

Faculty of Science-Chemistry

CH04 Pharmaceutical Chemistry

CH 86 04 02 -Advanced Pharmaceutical Operations and Dispensing

(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 the constituents of castor oil?

2. Name the important drugs obtained from Vasaka.

3. What are the pharmaceutical uses of talc?

4. Give an example for chemical incompatibility.

5. Give a brief account of the licencing authority of drugs in India.

6. What do you mean by diazotisation titrations?

7. What is electrophoresis?

8. Write a short note on non-aqueous titrations in pharmaceutical analysis.

9. List the major applications of mass spectrometry in pharmaceutical analysis.

10. Give a brief account of eucalyptus oil.

(8 x 1 = 8)

Section B

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

11. Write a note on the extraction of drugs from a) senna and b) cinchona.

12. Write notes on the preparation of pills, tablets and capsules.

13. Give a brief description of B.P. and I.P.

14. Write a note on patenting of pharmaceuticals in India.

15. Discuss the applications of extraction methods in pharmaceutical analysis.

16. Write a note on kidney function tests.

17. Give an account of radiopharmaceuticals.

18. Discuss the uses of gum tragacanth, agar agar and gelatinin pharmacy.

(**6 x 2 = 12**)

Section C

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

19. Discuss the applications of drugs obtained from the following plants and their extraction, i) cannabis, ii) ipecacuanha, iii) rauwolfia, iv) liquorice and v) ginger.

b) Give an account of fixed oils and essential oils used in pharmacy.

20. Discuss different drug delivery systems with special mention to site specific drug delivery systems in cancer chemotherapy, to brain and CNS, to kidney and urinary tract.

21. Give an account of rules regarding import, manufacture, storage, packing and labelling and sale of drugs and cosmetics based on The Drugs and Cosmetic Act.

22. a) Discuss the Applications of AAS, UV-Vis spectroscopy, IR-spectroscopy and NMR spectroscopy in pharmaceutical analysis.

b) Write a note on the diagnosis of Heart diseases.

(**2 x 5 = 10**)

QP Code **Reg. No. …..**

Name ……

M. Sc Pharmaceutical Chemistry Degree (C.S.S) Examination, ……

Fourth Semester

Faculty of Science- Chemistry

CH04 Pharmaceutical Chemistry

CH 86 04 03-MEDICINAL CHEMISTRY

(2019 admissions onwards)

Time: Three hours Max. Weight: 30

Section- A

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

1. 1. Give the name and structure of any two cardiotonic drugs.
2. Give two examples of adrenergic stimulants. Give its uses.
3. Write the mechanism of action of acyclovir.
4. Explain the action and pharmacological uses of pilocarpine.
5. Give the structure and use of chloramphenicol.
6. What are the important drugs used in the treatment of amoebiasis.
7. Suggest two drugs used in the treatment of tuberculosis with their structures.
8. Write the mechanism of action of cyclophosphamide as alkylating agent in cancer therapy.
9. What are curare form drugs? Give two examples.
10. What is the biological significance of H_1-receptor? **(8 x 1 = 8)**

Section B

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

11. Write short notes on anticholinesterases.
12. Discuss the chemistry of calcium channel blockers. Give the synthesis of verapamil.
13. Write notes on macrolide antibiotics specifying the mode of action.
14. What is the use of clotrimazole? Give its structure. What are its side effects?

15. Discuss folic acid antagonist with a suitable example.

16. Write notes on Antiparkinson's agents.

17. What are purgatives? Explain the different classes of purgatives citing suitable examples.

18. What are expectorants? Explain their chemistry giving examples. (**6 x 2 = 12**)

Section C

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

19. Discuss the chemistry and mode of action of adrenergic stimulants. Give the synthesis of salbutamol and propranolol.

20. Give an account of mechanism of action and metabolites of nitrates as antianginal agents? Give two examples with their synthesis.

21. What are local anaesthetics? What are its various classes? Explain with structure, chemistry and application.

22. a) Outline the chemistry of various categories of drugs used as antineoplastic agents.

    b) Explain the different categories of drugs used as antifungal agents with their mechanism of action.

(2 x 5 = 10)