POST GRADUATE AND RESEARCH DEPARTMENT OF CHEMISTRY MAHARAJA'S COLLEGE, ERNAKULAM

(A Government Autonomous College
Re-accredited by NAAC with 'A' grade
Centre for Excellence under Govt. of Kerala
Identified by UGC as College with Potential for Excellence)

CHOICE BASED CREDIT SYSTEM

SCHEME & SYLLABI FOR POST GRADUATE PROGRAMMES IN CHEMISTRY

2016

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FOREWORD

The Board of Studies in Chemistry take this opportunity to express our deep appreciation to all academicians and professionals who participated in the series of workshops organised by the Board for restructuring curriculum and syllabi of the PG courses in Chemistry - M.Sc Chemistry, M.Sc Analytical Chemistry, M.Sc Pharmaceutical Chemistry and M.Sc Applied Chemistry. We express our profound gratitude to the Honourable Vice-Chancellor, Pro-Vice Chancellor, Members of the Syndicate and Members of the Academic Council, Mahatma Gandhi University, for their sincere co-operation and guidance for completion of this work. Our special thanks are due to Chairman and members of the Governing Council, Chairman and members of the Academic Council, Maharaja's College, Ernakulam.

We also extend our gratitude to Prof. (Dr). K. K. Mohammed Yusuff, Professor (Retd.), Department of Applied Chemistry, Cochin University of Science and Technology, Prof. (Dr). S. Sugunan, Professor (Retd.), Department of Applied Chemistry, Cochin University of Science and Technology, Prof. (Dr). K. Girish Kumar, Professor, Department of Applied Chemistry, Cochin University of Science and Technology, Prof. (Dr). K. Sreekumar, Professor, Department of Applied Chemistry, Cochin University of Science and Technology, Dr. E. Prasad, Associate Professor, Department of Chemistry, IIT, Madras, Dr. Kochubaby Manjooran, Dy.Manager (Energy and Envt), BPCL, Kochi Refinery, Sri. M. G. Rajagopalan, Associate Professor(Retd.) Maharaja's College, Ernakulam, Smt. K. T. Geethabali, Associate Professor (Retd.), Maharaja's College, Ernakulam, Dr. T. Narayanan, Associate Professor (Retd.), Maharaja's College, Ernakulam, and Dr. Lissamma Koshy,. Associate Professor (Retd.), Maharaja's College, Ernakulam who were entrusted with the responsibility as experts for the revision of the syllabus of different subjects. The Board of Studies in Chemistry expresses the whole hearted gratitude to all those who have helped in this endeavour.

The task of preparing the curricula and syllabi and bringing it out in the present form for all the four M.Sc courses was not simple but it was possible with dedicated efforts and wholehearted support and involvement of all the members of the BOS and the faculty members of the Department of Chemistry. I would like to express my sincere thanks to all my fellow members of BOS and the faculty members of the Department of Chemistry for all their help, cooperation, encouragement, active participation and useful suggestions for the completion of syllabus.

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  Assistant Professor
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  Assistant Professor

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  Head of the Department
  Associate Professor
- **Dr. P V Joseph**
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  Assistant Professor
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  Associate Professor
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  Assistant Professor

PROGRAMME STRUCTURE

Examination

- There shall be end semester examination at the end of each semester.
- The answers must be written in English except for those coming under Faculty of Languages.
- Practical examinations shall be conducted by the college at the end of even semesters only.
- Project evaluation and Viva -Voce shall be conducted at the end of the programme only.
- Practical examination, Project evaluation and Viva-Voce shall be conducted by two external examiners.

END-Semester Examination

- The examinations shall normally at the end of each semester. There shall be one end-semester examination of 3 hours duration in each lecture based course and practical course.
- A question paper may contain short answer type/annotation, short essay type questions/problems and long essay type questions.

Evaluation and Grading

Evaluation

The evaluation scheme for each course shall contain two parts; (a) in-semester evaluation and (b) end-semester evaluation. 20 marks shall be given to in-semester evaluation and the remaining 80 marks to end-semester evaluation. Both in-semester and end semester evaluation shall be carried out by using in mark system. Both internal and external marks are to be mathematically rounded to the nearest integer.

Internal evaluation

The internal evaluation shall be based on predetermined transparent system involving periodic written tests, assignments, seminars and attendance in respect of theory courses and based on written tests, lab skill/records/viva and attendance in respect of practical courses. The marks assigned to various components for in-semester evaluation is as follows.

Components of In-semester Evaluation (For theory)

Components	Component Marks
Assignment	4
Seminar	4
Two Test papers*	8
Attendance	4
Total	20

*Marks of Test Papers shall be the average

Components of In-semester Evaluation (For Practical)

Components	Component Marks
Attendance	4
Laboratory Involvement	4
Written/Lab Test	4
Record*	4
Viva	4
Total	20

*Marks awarded to Record should be related to number of experiments recorded

Components of In-semester Evaluation (For Project)

Components	Marks
Topic/Area selected	2
Experimentation/Data collection	4
Punctuality	2
Compilation	4
Content	4
Presentation	4
Total	**20**

a) Evaluation of Attendance

% of attendance	Mark
95 and above	4
85 to 94	3
80 to 84	2
75 to 79	1
< 75	0

(Decimals are to be rounded to the next higher whole number)

b) Evaluation of Assignment

Components	Marks
Punctuality	1
Content	1
Conclusion	1
Reference/Review	1
Total	**4**

c) Evaluation of Seminar

Components	Marks
Content	1
Presentation	2
Reference/Review	1
Total	**4**

To ensure transparency of the evaluation process, the in-semester marks awarded to the students in each course in a semester shall be published on the notice board at least one week before the commencement of external examination. There shall not be any chance for improvement for in semester marks.

The course teacher and the faculty advisor shall maintain the academic record of each student registered for the course and a copy should be kept in the college for at least one year for verification.

End-Semester Evaluation:

The end-semester evaluation in theory courses is to be conducted by the college with question papers set by external experts. The answers must be written in English except those for the Faculty of Languages. The evaluation of the answer scripts shall be done by examiners based on a well-defined scheme of valuation. The end-semester evaluation shall be done immediately after the examination preferably through Centralized Valuation.

Photocopies of the answer scripts of the external examination shall be made available to the students for scrutiny on request and revaluation/scrutiny of answer scripts shall be done as per the request of the candidate by paying fees.

The question paper should be strictly on the basis of model question paper set by BOS and there shall be a combined meeting of the question paper setters for scrutiny and finalization of question paper. Each set of question should be accompanied by its answer scheme for valuation.

Pattern of Questions

The question setter shall ensure that questions to course should satisfy weightage to objectives and weightage to difficulty levels.

Weightage to Objectives	
Objectives	**%**
Understanding	25
Critical Evaluation	50
Application	25

Weightage to difficulty levels	
Level of difficulty	**%**
Easy	20
Average	60
Difficult	20

Question paper setters shall also submit a detailed scheme of evaluation along with the question paper. A question paper shall be a judicious mix of objective type, short answer type, short essay type /problem solving type and long essay type questions.

Pattern of questions for end semester examination

	Total no. of questions	Number of questions to be answered	Marks of each question	Total marks
	12	10	2	20
	10	6	5	30
	4	2	15	30
TOTAL	**26**	**18**	x	**80**

Grades for Courses

For all courses (theory & practical), grades are given on a 10-point scale based on the total percentage of marks ***(ISA+ESA)*** as given below

Percentage of Marks	Grade	Grade Point (GP)
95 and above	S Outstanding	10
85 to below 95	A^+ Excellent	9
75 to below 85	A Very Good	8
65 to below 75	A- Good	7
55 to below 65	B^+ Above Average	6
50 to below 55	B Average	5
40 to below 50	C Pass	4
Below 40	F Fail	0
	Ab Absent	0

Credit Point and Credit Point Average

Credit Point (CP) of a course is calculated using the formula

CP = C × GP, where C = Credit; GP = Grade point

Semester Grade Point Average (SGPA) of a Semester is calculated using the formula

SGPA= TCP/TC, where TCP = Total Credit Point of that Semester

TC = Total Credit of that Semester

Cumulative Grade Point Average (CGPA) of a Programme is calculated using the formula

CGPA = ∑(TCP ×TC)÷∑TC

CGPA shall be rounded off to two decimal places

Grades for the different semesters and overall programme are given based on the corresponding CPA as shown below:

GPA	Grade
Equal to 9.5 and above	***S Outstanding***
Equal to 8.5 and below 9.5	***A+ Excellent***
Equal to 7.5 and below 8.5	***A Very Good***
Equal to 6.5 and below 7.5	***A- Good***
Equal to 5.5 and below 6.5	***B+ Above Average***
Equal to 5.0 and below 5.5	***B Average***
Equal to 4.0 and below 5.0	***C Pass***
Below 4.0	***F Failure***

M.Sc. CHEMISTRY

M.Sc. CHEMISTRY

	Code	Course	Hours/ week	Total Hours	Credit	Marks		
						Internal	External	Total
Semester 1	PG1CHE C01	Inorganic Chemistry-I (Coordination & Nuclear Chemistry)	4	72	4	20	80	100
	PG1CHE C02	Organic Chemistry-I (Structure, Reactivity & Stereochemistry)	4	72	4	20	80	100
	PG1CHE C03	Theoretical Chemistry-I (Quantum Chemistry and Group Theory)	4	72	4	20	80	100
	PG1CHE C04	Physical chemistry- I (Kinetic Theory, Thermodynamics and Statistical Thermodynamics)	3	54	3	20	80	100
	PG2CHE P01	Inorganic Chemistry Practical–1	3	54	Evaluation at the end of second semester			
	PG2CHE P02	Organic Chemistry Practical-1	3	54				
	PG2CHE P03	Physical Chemistry Practical -1	4	72				
		Total	**25**	**450**	**15**			
Semester 2	PG2CHE C05	Inorganic Chemistry-II (Bioinorganic & Organometallic Chemistry)	4	72	4	20	80	100
	PG2CHE C06	Organic Chemistry- II (Reaction Mechanism)	4	72	4	20	80	100
	PG2CHE C07	Theoretical Chemistry – II (Chemical Bonding and Computational Chemistry)	4	72	4	20	80	100
	PG2CHE C08	Physical chemistry- II (Molecular Spectroscopy)	3	54	3	20	80	100
	PG2CHE P01	Inorganic Chemistry Practical–1	3	54	3	20	80	100
	PG2CHE P02	Organic Chemistry Practical-1	3	54	3	20	80	100
	PG2CHE P03	Physical Chemistry Practical -1	4	72	4	20	80	100
		Total	**25**	**450**	**25**			

Semester 3	PG3CHE C09	Inorganic chemistry-III (Solid State Chemistry)	4	72	4	20	80	100
	PG3CHE C10	Organic chemistry- III (Organic Syntheses)	4	72	4	20	80	100
	PG3CHE C11	Physical chemistry- III (Chemical Kinetics, Surface Chemistry and Photochemistry)	4	72	4	20	80	100
	PG3CHE C12	Spectroscopic Methods in Chemistry	3	54	3	20	80	100
	PG4CHE P04	Inorganic Chemistry Practical–2	3	54	Evaluation at the end of fourth semester			
	PG4CHE P05	Organic Chemistry Practical-2	3	54				
	PG4CHE P06	Physical Chemistry Practical -2	4	72				
		Total	**25**	**450**	**15**			
Semester 4	PG4CHE E01	Elective –I Inorganic Chemistry - IV (Advanced Inorganic Chemistry)	5	90	4	20	80	100
	PG4CHE E02	Elective –II Organic Chemistry-IV (Advanced Organic Chemistry)	5	90	4	20	80	100
	PG4CHE E03	Elective –III Physical Chemistry- IV (Advanced Physical Chemistry)	5	90	4	20	80	100
	PG4CHE E04	Elective –IV Polymer Chemistry	5	90	4	20	80	100
	PG4CHE E05	Elective –V Analytical Chemistry	5	90	4	20	80	100
	PG4CHE P04	Inorganic Chemistry Practical–2	3	54	3	20	80	100
	PG4CHE P05	Organic Chemistry Practical-2	3	54	3	20	80	100
	PG4CHE P06	Physical Chemistry Practical -2	4	72	3	20	80	100
	PG4CHE D01	Project			2	20	80	100
	PG4CHE V01	Viva			2	20	80	100
		Total	**25**	**450**	**25**			
Grand Total					**80**			

SEMESTER 1

PG1CHE C01 INORGANIC CHEMISTRY – I

(COORDINATION & NUCLEAR CHEMISTRY)

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

Module 1: Coordination Chemistry- Structural Aspects and Bonding (18 Hrs)

1.1 Classification of complexes based on coordination numbers and possible geometries. σ and π bonding ligands such as CO, NO, CN^-, R_3P and Ar_3P.

1.2 Splitting of *d* orbitals in octahedral, tetrahedral, square planar, square pyramidal and trigonal 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 with and without π-bonding, experimental evidences for π-bonding

Module 2: Kinetics and Mechanism of Reactions in Metal Complexes (18 Hrs)

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

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

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

Module 3: Organometallic Compounds- Synthesis, Structure and Bonding (18 Hrs)

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

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

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

Module 4: Electron deficient compounds (9 Hrs)

Electron deficient compounds – synthesis, reactions, structure and bonding. Boron hydrides, styx numbers, Boron cluster compounds.
Wade's rule, Hydroborate anions, Organoboranes and hydroboration, Polyhedral anions, Carboranes, Metalloboranes, Borazines and Borides.

Module 5: Nuclear Chemistry (9 Hrs)

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

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

5.3 Analytical applications of radioisotopes- radiometric titrations, kinetics of exchange reactions, measurement of physical constants including diffusion constants, neutron activation analysis, prompt gamma neutron activation analysis and neutron absorptiometry.

5.4 Applications of radio isotopes in industry, medicine, autoradiography, radiopharmacology, radiation safety precaution, nuclear waste disposal.

5.5 Radiation chemistry of water and aqueous solutions- Fricke solution, Ceric ammonium solution. Measurement of radiation doses. Relevance of radiation chemistry in biology, organic compounds and radiation polymerization.

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PG1CHE C02 ORGANIC CHEMISTRY - I

(STRUCTURE, REACTIVITY & STEREOCHEMISTRY)

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

Module 1: MO Theory and Aromaticity (9 Hrs)

1.1 Review of basic concepts in organic chemistry: bonding, hybridization, MO picture (allyl system, 1,3-butadiene and benzene), inductive effect, electromeric effect, resonance effect, hyperconjugation, steric effect. Bonding weaker than covalent bonds.

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

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

Module 2: Investigation of Organic Reaction Mechanisms (9 Hrs)

Energy profiles, Methods of determining reaction mechanisms, Kinetic and thermodynamic control of reactions. The Hammond postulate. Principle of microscopic reversibility. Marcus theory. The Hammett equation and its applications. Taft equation. Linear free energy relationships. Solvent polarity and parameters. Y, Z and E parameters and their applications. Primary and secondary kinetic isotope effects. Salt effects and special salt effects in SN reactions. Solvent effect. Bulk and specific solvent effects. Introduction to carbon acids - pKa of weak acids, kinetic and thermodynamic acidity. Phase transfer catalysis and its applications. Steric effects. HSAB principle and its applications in organic reactions.

Module 3: Review of Organic Reaction Mechanisms (18 Hrs)

3.1 Review of organic reaction mechanisms with special reference to nucleophilic and electrophilic substitution at aliphatic carbon (S_N1, S_N2, S_Ni, S_E1, S_E2, addition-elimination and elimination-addition sequences), elimination (E1 and E2). Elimination vs substitution.

3.2 A comprehensive study on the effect of substrate, reagent, leaving group, solvent and neighbouring group on nucleophilic substitution (S_N2 and S_N1) and elimination (E1 and E2) reactions.

3.3 Addition reactions (regioselectivity- Markovnikov's addition- carbocation mechanism, anti-Markovnikov's addition- radical mechanism).

3.4 Mechanism of electrophilic and nucleophilic aromatic substitution reactions with examples. Arenium ion intermediates. S_N1, S_NAr, $S_{RN}1$ and Benzyne mechanisms.

3.5 Catalysis by acids, bases and nucleophiles with examples from acetal, cyanhydrin and ester formation and hydrolysis reactions- $A_{AC}2$, $A_{AC}1$, $A_{AL}1$, $B_{AC}2$ and $B_{AL}1$ mechanisms.

Module 4: Stereochemistry of Organic Compounds (18 Hrs)

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

4.2 Stereoisomerism: Definition based on symmetry and energy criteria, configurational and conformational stereoisomers.

4.3 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 C_n, molecules with more than one center of chirality, definition of diastereoisomers, constitutionally symmetrical and unsymmetrical chiral molecules, erythro and threo nomenclature.

4.4 Axial, planar and helical chirality with examples, stereochemistry and absolute configuration of allenes, biphenyls, binaphthyls, ansa and cyclophanic compounds, spiranes, exocyclic alkylidene cycloalkanes.

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

4.6 Geometrical isomerism: Nomenclature, E-Z notation, methods of determination of geometrical isomers. Interconversion of geometrical isomers.

Module 5: Conformational Analysis (18 Hrs)

5.1 Conformational descriptors- factors affecting conformational stability of molecules. Conformational analysis of acyclic and cyclic systems: substituted ethanes, cyclohexane and its derivatives, decalins, adamantane, congressane, sucrose and lactose. Fused and bridged bicyclic systems.

5.2 Conformation and reactivity of elimination (dehalogenation, dehydrohalogenation, semipinacolic deamination and pyrolytic elimination- Saytzeff and Hofmann eliminations), substitution and oxidation of 2° alcohols. Chemical consequence of conformational equilibrium - Curtin Hammett principle. Chiral drugs.

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PG1CHE C03 THEORETICAL CHEMISTRY – I

(QUANTUM CHEMISTRY AND GROUP THEORY)

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

Module 1: Formulation of Quantum Chemistry (18 Hrs)

1.1 Mathematical Concepts (5 Hrs)

Co-ordinate systems: Cartesian, Cylindrical polar and Spherical polar coordinates and their relationships. Complex numbers: definition, Complex conjugate, absolute value of a complex number, complex functions. Operator algebra: linear and nonlinear operators, Hermitian operators, del and del-squared operators. Eigen function and eigen values of an operator, Eigen value equation, Eigen functions of Commuting operators. Well behaved functions, Normalized and Orthogonal functions.

1.2 Evolution of Quantum Mechanics (5 Hrs)

Failure of classical mechanics: The black body radiation, Compton effect, photoelectric effect, atomic spectra. Need of quantum mechanics. Concept of matter wave, de Broglie relation and its experimental proof, Uncertainty principle and its consequences. Wave function and Born interpretation, Schrödinger's wave mechanics, Deduction of Schrodinger equation from classical wave equation.

1.3 Postulates of Quantum Mechanics (4 Hrs)

Detailed discussion of postulates: State function postulate. Operator postulate. Eigen value postulate. Expectation value postulate. Postulate of time dependent Schrodinger equation of motion, Conservative system and time-independent Schrodinger equation.

1.4 Quantum Mechanics of Translational Motion (4 Hrs)

Particle in one-dimension with infinite potential walls, particle in a three dimensional box- separation of variables- rectangular box and cubic box, degeneracy. Introduction to tunnelling with experimental evidence.

Module 2: Applications of Quantum Chemistry (18 Hrs)

2.1 Quantum Mechanics of Hydrogen-like Atoms (5 Hrs)

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

2.2 Quantum Mechanics of Vibrational Motion (5 Hrs)

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. Rodrigue's formula, Three dimensional harmonic oscillator.

2.3 Quantum Mechanics of Rotational Motion (5 Hrs)

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 Φ equation and its solution, wave functions in the real form. Non-planar rigid rotor (or particle on a sphere)-separation of variables, the Φ and the Θ equations and their solutions, Legendre and associated Legendre equations, Legendre and associated Legendre polynomials. Spherical harmonics (imaginary and real forms)- polar diagrams of spherical harmonics.

2.4 Orbital and Spin angular momentum (3 Hrs)

Quantisation of angular momentum, quantum mechanical operators corresponding to angular momenta, (L_x, L_y, L_z and L^2). Commutation relations between these operators. Spherical harmonics as eigen functions of angular momentum operators L_z and L^2. Space quantization. The postulate of spin by Uhlenbeck and Goudsmith, discovery of spin- Stern Gerlach experiment. Spin orbitals- construction of spin orbitals from orbital and spin functions.

Module 3: Molecular Symmetry and Mathematical group (18 Hrs)

3.1 Symmetry elements and symmetry operations. Conditions for a set of elements to form a group, sub groups, abelian and cyclic groups, Point groups. Multiplication of operations. Group multiplication table of C_{2v}, C_{2h} and C_{3v} groups (H_2O, Trans N_2F_2 and NH_3 as examples). Similarity transformation and classes in a group.

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

3.3 Reducible and Irreducible representations (IR). Reduction formula, reduction of reducible representation to IRs.

Module 4: Applications of Group Theory (18 Hrs)

4.1 The Great Orthogonality theorem. Rules derived from GOT (proof not required). Setting up of character table of C_{2v}, C_{3v}, C_{2h}, C_{4v} and C_3 groups. Direct product representations.

4.2 Applications in quantum mechanics, transition moment integral, vanishing of integrals. Jahn – Teller effect, Woodward – Hoffmann rules.

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

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

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

PG1CHE C04 - PHYSICAL CHEMISTRY - I

(KINETIC THEORY, THERMODYNAMICS AND STATISTICAL THERMODYNAMICS)

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

Module 1: Kinetic theory **(9 Hrs)**

Kinetic theory of gases, 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, transport properties of gases. Viscosity, thermal conductivity and diffusion. Determination of viscosity of gases. Influence of temperature and pressure on transport properties.

Module 2: Classical Thermodynamics **(18 Hrs)**

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

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

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

2.4 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.

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

2.6 Chemical affinity and thermodynamic functions, effect of temperature and pressure on chemical equilibrium- van't Hoff reaction isochore and isotherm.

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

2.8 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, and three pairs of partially miscible liquids.

Module 3: Irreversible Thermodynamics and Bioenergetics (9 Hrs)

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

Module 4: Statistical Thermodynamics (18 Hrs)

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

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

References

[1] P.W. Atkins, Physical Chemistry, ELBS, 1994.

[2] K.J. Laidler, J.H. Meiser, B.C. Sanctuary, Physical Chemistry, 4^{th} Edn., Houghton Mifflin, 2003.

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[13] R.K. Murray, D.K. Granner, P. A. Mayes, V.W. Rodwell, Harper's Biochemistry, Tata McGraw Hill, 1999.

SEMESTER 2

PG2CHE C05 INORGANIC CHEMISTRY- II

(BIOINORGANIC & ORGANOMETALLIC CHEMISTRY)

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

Module 1: Acids, Bases and Non-aqueous solvents (9 Hrs)

1.1 Acid base concept in non-aqueous media-HSAB concept, solvent effect, linear free energy relationship- mechanism and method of determination.

1.2 Reaction in non-aqueous solvents. Ammonia- solution of metals in liquid ammonia. Protonic solvents: anhydrous sulphuric acid, hydrogen halide. Aprotic solvents: non-polar solvents, non-ionizable polar solvents. Polar solvents undergoing autoionization. Liquid halogen, Inter halogen compounds, oxy halides, dinitrogen tetroxide, sulphur dioxide.

Module 2: Bioinorganic Compounds (18 Hrs)

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

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

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

Module 3: Spectral and Magnetic Properties of Metal Complexes (18 Hrs)

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

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

3.3 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.

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

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

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

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

Module 5: Stereochemistry of Coordination Compounds (9 Hrs)

5.1 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.

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

Module 6: Reactions of Organometallic Compounds (9 Hrs)

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

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

6.3 Rearrangement reactions, redistribution reactions, fluxional isomerism.

References

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

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

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PG2CHE C06 ORGANIC CHEMISTRY - II

(REACTION MECHANISM)

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

Module 1: Chemistry of Carbocations (9 Hrs)

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

1.2 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, Demjanov rearrangement. Oxymercuration, halolactonisation.

Module 2: Chemistry of Carbanions (18 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, Kinetic and thermodynamic enolates- Lithium and boron enolates in Michael and aldol reactions, alkylation and acylation of enolates. Chemistry of enamines, Stork-Enamine reaction.

2.2 Nucleophilic additions to carbonyls groups. Reactions involving carbanions-mechanisms of Claisen, Dieckmann, Knoevenagel, Stobbe, Darzen and acyloin condensations, Shapiro reaction and Julia elimination. Favorskii rearrangement.

2.3 Reactions of carbonyl compounds: oxidation, reduction (Clemmensen and Wolff-Kishner), addition reactions (addition of cyanide, ammonia, alcohol), Aldol condensation, Cannizzaro reaction, addition of Grignard reagent.

2.4 Structure and reactions of α, β- unsaturated carbonyl compounds involving electrophilic and nucleophilic addition- Michael addition, Mannich reaction, Robinson annulation.

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

Module 3: Carbenes, Carbenoids, Nitrenes and Arynes (9 Hrs)

3.1 Generation, structure and reactions of carbenes. Rearrangement reactions of carbenes: Wolff rearrangement, generation and reactions of ylids by carbenoid decomposition.

3.2 Structure, generation and reactions of nitrenes. Hoffmann, Curtius, Lossen, Schmidt and Beckmann rearrangement reactions.

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

Module 4: Radical Reactions (9 Hrs)

4.1 Generation and detection 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. Autoxidation.

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

Module 5: Concerted reactions (18 Hrs)

5.1 Symmetry properties of molecular orbitals of ethylene and conjugated systems with three or more atoms, Woodward – Hoffmann rule, Conservation of orbital symmetry and stereo chemical courses.

5.2 Pericyclic reactions like Electrocyclic (butadiene-cyclobutene and hexatriene-cyclohexadiene interconversions), Cycloadditions (2+2) & (4+2), Sigmatropic (1,3), (1,5) and (3,3), Cheletropic including Cheletropic eliminations and Ene reaction with stereo chemical aspects.

5.3 Diels- Alder reactions with stereochemical aspects.

5.4 Analysis of Pericyclic Reactions. (i) FMO method (ii) Orbital- correlation method and (iii) PMO method.

5.2 Highlighting pericyclic reactions in organic synthesis such as Claisen, Cope, Mislow-Evans, Wittig and Sommelet-Hauser rearrangements. dipolar cycloaddition (introductory). Unimolecular pyrolytic elimination reactions, decomposition of

cyclic azo compounds, β-eliminations involving cyclic transition states such as N-oxides, acetates and xanthates.

Module 6: Organic Photochemistry (9 Hrs)

6.1 Photochemical processes. Energy transfer. Jablonski diagram, sensitization and quenching. Singlet and triplet states and their reactivity.

6.2 Photoreactions of carbonyl compounds, enes, dienes and arenes. Norrish reactions of acyclic ketones. Patterno-Buchi, Barton, Photo-Fries and Di-л methane rearrangements. Photoreactions of Vitamin D. Photosynthesis and photochemistry of vision. Singlet oxygen generation and their reactions**.**

References

[1] R. Bruckner, Advanced Organic Chemistry: Reaction Mechanism, Academic Press, 2002.

[2] F.A. Carey, R.A. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5^{th} Edn., Springer Science & Business Media, 2007.

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PG2CHE C07 THEORETICAL CHEMISTRY - II

(CHEMICAL BONDING AND COMPUTATIONAL CHEMISTRY)

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

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

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

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

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

Module 2: Chemical Bonding (18 Hrs)

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

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

2.3 Hybridization, quantum mechanical treatment of sp, sp^2 and sp^3 hybridisation. Semiempirical MO treatment of planar conjugated molecules, Hückel Molecular

Orbital (HMO) theory of ethene, allyl systems, butadiene and benzene. Calculation of charge distributions, bond order and free valency.

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

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

Module 4: Computational Chemistry (18 Hrs)

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

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

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

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

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

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

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

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

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

Module 5: Computational Chemistry Calculations (9 Hrs)

5.1 Molecular geometry input- Cartesian coordinates and internal coordinates, Z-matrix. Z-matrix of: single atom, diatomic molecule, non-linear triatomic molecule, linear triatomic molecule, polyatomic molecules like ammonia, methane, ethane and butane. General format of GAMESS/Firefly input file. GAMESS/Firefly key word for: basis set selection, method selection, charge, multiplicity, single point energy calculation, geometry optimization, constrained optimization and frequency calculation.

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

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

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[1] I.N. Levine, Quantum Chemistry, 6th Edn., Pearson Education, 2009.

[2] D.A. McQuarrie, Quantum Chemistry, University Science Books, 2008.

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

Softwares

Molecular Mechanics:

01. **Arguslab** available from www.arguslab.com/
02. **Tinker** available from www.dasher.wustl.edu/ffe/

Ab initio, semiempirical and dft:

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

Graphical User Interface (GUI):

01. **Gabedit** available from http://gabedit.sourceforge.net/
02. **wxMacMolPlt** available from http://www.scl.ameslab.gov/MacMolPlt/
03. **Avogadro** from http://avogadro.openmolecules.net/wiki/Get_Avogadro

PG2CHE C08 PHYSICAL CHEMISTRY - II

(MOLECULAR SPECTROSCOPY)

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

Module 1: Microwave and Infrared Spectroscopy (18 Hrs)

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

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

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

Module 2: Electronic, Mossbauer and Raman spectroscopy (18 Hrs)

2.1 Electronic spectroscopy: Term symbols of diatomic molecules, electronic spectra of diatomic molecules, selection rules, vibrational coarse structure and rotational fine structure of electronic spectrum, Franck-Condon principle, predissociation, calculation of heat of dissociation, Birge and Sponer method, electronic spectra of polyatomic molecules, spectra of transitions localized in a bond or group, free electron model.

Different types of lasers- solid state lasers, continuous wave lasers, gas lasers and chemical laser, frequency doubling, applications of lasers, introduction to UV and X-ray photoelectron spectroscopy.

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

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

Module 3: Resonance Spectroscopy (18 Hrs)

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

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

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

3.4 An elementary study of NQR spectroscopy.

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.

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[13] D.N. Sathyanarayana, Introduction to Magnetic Resonance Spectroscopy ESR, NMR, EQR, I.K. International Publishing House Pvt. Limited, 2009.

SEMESTERS 1 AND 2

PG2CHE P01 INORGANIC CHEMISTRY PRACTICAL – 1

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

PART I

Separation and identification of four metal ions of which two are rare/ less familiar such as Tl, W, V, Se, Te, Ti, Ce, Th, Zr, U, Mo and Li and common cations - 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+}, Co^{2+}, Ni^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}, Mg^{2+}, Li^+, Na^+, K^+, NH_4^+ (interfering acid radicals are not present). Confirmation by spot test (Minimum **8** mixtures are to be recorded).

PART II

1. Argentometric estimation of chlorides
2. Cerimetry – Fe(II) and nitrate
3. Potassium iodate – iodide estimation of Sn(II)

PART III

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

PART IV

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

1. Tris (thiourea) copper (I) complex
2. Potassium tris (oxalate) aluminate (III)
3. Tetrammine copper (II) sulphate
4. Mercury tetra thiocyanato cobaltate (III)

References

[1] A.I. Vogel, A Text Book of Qualitative Inorganic Analysis Including Elementary Instrumental Analysis, 3rd Edn., ELBS.

[2] G. Svelha, Text Book of Vogel's Macro and Semi-micro Inorganic Analysis, revised, Orient Longman.

[3] V.V. Ramanujam, Inorganic Semi micro Qualitative Analysis, The National Publishing Co., Chennai.

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

PG2CHE P02 ORGANIC CHEMISTRY PRACTICAL - 1

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

PART I

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

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

PART II

A. Separation of organic binary mixtures:- 1. Quantitative separation of a mixture of two components by solvent extraction 2. Purification of the separated samples by distilling and crystallization. 3. Determination of physical constants of separated and purified samples (No need of bifunctional compounds).

B. Separation of organic mixtures by TLC and calculation of R_f values.

C. Separation/purification of organic mixtures by column chromatography.

PART III

Drawing the structures of organic molecules and reaction schemes and mechanisms by ChemDraw, SymyxDraw and Chemsketch.

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

PART IV- Viva voce

References

[1] A.I. Vogel, A Textbook of Practical Organic Chemistry, Longman, 1974.

[2] A.I. Vogel, Elementary Practical Organic Chemistry, Longman, 1958.

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

[4] R. Adams, J.R. Johnson, J.F. Wilcox, Laboratory Experiments in Organic Chemistry, Macmillan, 1979.

[5] A.I. Vogel, A.R. Tatchell, B.S. Furnis, A.J. Hannaford, P.W.G. Smith, Vogels Text Book of Practical Organic Chemistry, 5th Edn., Prentice Hall, 1989.

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[7] N.K.Vishnoi, Advanced Practical Organic Chemistry, 3rd Edn., Vikas Publishing House, 2009.

[8] J.B. Cohen, Practical Organic Chemistry, Mc Graw Hill.

[9] C.E Bella and DF Taber, Organic Chemistry Laboratory, Thomson.

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[11] Monograph on green laboratory experiments, DST, Govt of India.

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PG2CHE P03 PHYSICAL CHEMISTRY PRACTICAL - 1

Credit: 4 **Contact Lab Hours: 72+72 =144**

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

Part A

I. Adsorption

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

II. Phase diagrams

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

III. Distribution law

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

IV. Surface tension

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

Part B

Computational Chemistry Experiments

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

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

References

[1] J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.

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

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

[4] GAMESS documentation available from: http://www.msg.ameslab.gov/gamess/documentation.html.

SEMESTER 3

PG3CHE C09 INORGANIC CHEMISTRY- III

(SOLID STATE CHEMISTRY)

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

Module 1: Solid State Chemistry **(18 Hrs)**

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

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

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

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

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

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

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

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

Module 3: Inorganic Chains and Rings (18 Hrs)

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

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

Module 4: Organometallic Polymers (9 Hrs)

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

Module 5: Chemistry of Materials (9 Hrs)

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

References

[1] L.V. Azaroff, Introduction to Solids, Mc Graw Hill, 1984.

[2] A.R. West, Solid State Chemistry and its Applications, Wiley-India, 2007.

[3] D.K. Chakrabarty, Solid State Chemistry, New Age Pub., 2010.

[4] D.M. Adams, Inorganic Solids: An Introduction to Concepts in Solid State Structural Chemistry, Wiley, 1974.

[5] C.N.R. Rao, K.J. Rao, Phase Transitions in Solids, McGraw Hill, 2010.

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[8] J.E. Huheey, E.A. Keiter, R.L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Harper Collins College Pub.,1993, 33.

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

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

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

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

[13] B.D. Guptha, A.J Elias, Basic Organometallic Chemistry, Universities Press, 2010.

PG3CHE C10 ORGANIC CHEMISTRY - III

(ORGANIC SYNTHESES)

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

Module 1: Retrosynthetic Analysis **(9 Hrs)**

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

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

Module 2: Organometallics **(9 Hrs)**

Preparation and applications in organic synthesis of (i) Organo lithium compounds and addition to −C=O, −COOH and –$CONR_2$ (ii) Lithium dialkylcuprates (Gilman reagent) and reaction with alkyl halides, aryl halides and enones (iii) Alkynyl Cu(I) reagents and Glaser coupling (iv) Dialkyl cadmium compounds and (v) Benzenetricarbonyl chromium and reaction with carbanions.

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

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

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

Module 4: Modern Synthetic Methods and Reagents (18 Hrs)

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

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

Module 5: Construction of Carbocyclic and Heterocyclic Ring System (9 Hrs)

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

5.2 Formation of heterocyclic rings: 5- and 6-membered and condensed ring heterocyclic compounds with one or more than one hetero atom like N, S or O - pyrrole, furan, thiophene, pyridine, imidazole, thiazole, oxazole, pyrimidines, purines, quinoline and isoquinoline.

Module 6: Protecting Group Chemistry (9 Hrs)

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

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

6.3 Role of trimethyl silyl group in organic synthesis.

References

[1] M.B. Smith, Organic Synthesis, 3rd Edn., Wavefunction Inc., 2010.

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

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[13] F. Rutjes, V.V. Fokin, K.B. Sharpless, Click Chemistry: In Chemistry, Biology and Macromolecular Science, Wiley, 2012.

PG3CHE C11- PHYSICAL CHEMISTRY- III

(CHEMICAL KINETICS, SURFACE CHEMISTRY AND PHOTOCHEMISTRY)

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

Module 1: Chemical Kinetics **(18 Hrs)**

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

1.2 Lindemann-Hinshelwood mechanism, qualitative idea of RRKM theory, chain reactions: free radical and chain reactions, steady state treatment, Kinetics of H_2-Cl_2 and H_2-Br_2 reactions, Rice-Herzfeld mechanism, branching chains H_2-O_2, Semonov-Hinshelwood mechanism of explosive reactions, mechanisms of step-growth, ionic and addition polymerization, kinetics of anionic and cationic polymerization.

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

1.4 Reactions in solution: factors determining reaction rates in solutions, effect of dielectric constant and ionic strength, cage effect, Bronsted-Bjerrum equation, primary and secondary kinetic salt effect, influence of solvent on reaction rates, significance of volume of activation, linear free energy relationship, kinetic isotope effect.

Module 2: Surface Chemistry **(18 Hrs)**

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

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

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

Module 3: Catalysis (9 Hrs)

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

3.2 Enzyme catalysis and its mechanism, Michaelis-Menton equation, effect of pH and temperature on enzyme catalysis.

3.3 Mechanisms of heterogeneous catalysis: unimolecular and bimolecular surface reactions, mechanisms of catalyzed reactions like ammonia synthesis, Fischer-Tropsch reactions, hydrogenation of ethylene and catalytic cracking of hydrocarbons and related reactions.

Module 4: Colloids and Macromolecules (9 Hrs)

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

4.2 Macromolecules: Molecular mass- different averages, relation between different averages, calculation of different averages, methods of molecular mass determination- osmotic pressure, viscosity, sedimentation and light scattering methods.

Module 5: Photochemistry (18 Hrs)

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

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

5.3 Quenching of fluorescence and its kinetics, Stern-Volmer equation, concentration quenching, fluorescence and structure, delayed fluorescence, E-type and P-type, effect of temperature on emissions, photochemistry of environment, green house effect, two photon absorption spectroscopy, lasers in photochemical kinetics.

References

[1] J. Rajaram, J.C. Kuriakose, Kinetics and Mechanisms of Chemical Transformations, Macmillan India, 2000.

[2] K.J. Laidler, Chemical kinetics, 3rd Edn., Harper & Row, 1987.

[3] C. Kalidas, Chemical Kinetic Methods: Principles of Fast Reaction Techniques and Applications, New Age International, 2005.

[4] J.W. Moore, R.G. Pearson, Kinetics and Mechanisms, John Wiley & Sons, 1981.

[5] P.W. Atkins, Physical Chemistry, ELBS, 1994.

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

[7] A.W. Adamson, A.P. Gast, Physical Chemistry of Surfaces, 6th Edn., John Wiley & sons, 1997.

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[9] G. Aruldhas, Molecular structure and Spectroscopy, PHI Learning, 2007.

PG3CHE C12 SPECTROSCOPIC METHODS IN CHEMISTRY

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

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

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

1.2 Influence of substituent, ring size and strain on spectral characteristics. Solvent effect, Stereochemical effect, non-conjugated interactions.

1.3 Problems based on the above topics.

1.4 Chirooptical properties- ORD, CD, octant rule, axial haloketone rule, Cotton effect.

Module 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.

Module 3: Nuclear Magnetic Resonance Spectroscopy (18 Hrs)

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

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

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

3.4 2D NMR and COSY, HOMOCOSY and HETEROCOSY

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

3.6 Problems on spectral interpretation with examples.

Module 4: Mass Spectrometry (9 Hrs)

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

4.2 Problems on spectral interpretation with examples.

Module 5: Structure Elucidation Using Spectroscopic Techniques (9 Hrs)

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

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

References

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

[2] A.U. Rahman, M.I. Choudhary, Solving Problems with NMR Spectroscopy, Academic Press, 1996.

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

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

[6] H. Gunther, NMR Spectroscopy, 2nd Edn., Wiley, 1995.

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

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

[9] W. Kemp, Organic Spectroscopy, 2nd Edn., Macmillan, 1987.

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

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

[12] Online spectral databases including RIO-DB.

[13] P.S. Kalsi. Spectroscopy of Organic Compounds, 5th Edn., New Age International, 2004.

SEMESTER 4

ELECTIVE COURSES

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

PG4CHE E01 INORGANIC CHEMISTRY - IV

(ADVANCED INORGANIC CHEMISTRY)

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

Module 1: Applications of Group Theory (36 Hrs)

1.1 Transformation properties of atomic orbitals, hybridization schemes for σ and π bonding with examples, Symmetry Adapted Linear Combination of Atomic orbitals in tetrahedral, octahedral and sandwich complexes.

1.2 Ligand field theory-splitting of d orbitals in different environments using group theoretical considerations, construction of energy level diagrams, correlation diagrams, method of descending symmetry, formation of symmetry adapted group of ligands, M.O. diagrams, splitting terms for orbitals, energy levels, d-d transition-selection rules, vanishing integrals. Raman spectra of complexes with oxo anions as ligands, IR and Raman spectra using character tables in tetrahedral, octahedral and square planar complexes.

Module 2: Inorganic Spectroscopic Methods (9 Hrs)

2.1 Infrared and Raman Spectroscopy: structural elucidation of coordination compounds containing the following molecules/ions as ligands- NH_3, H_2O, CO, NO, OH^-, SO_4^{2-}, CN^-, SCN^-, NO_2^- and X^- (X=halogen).

2.2 Electron Paramagnetic Resonance Spectroscopy: EPR of d^1 and d^9 transition metal ions in cubic and tetragonal ligand fields, evaluation of g values and metal hyperfine coupling constants.

2.3 Mössbauer Spectroscopy: applications of Mössbauer spectroscopy in the study of Fe(III) complexes.

Module 3: Inorganic Photochemistry (9 Hrs)

3.1 Excited states, ligand field states, charge-transfer states and phosphorescence and fluorescence. Photochemical reactions-substitution and redox reactions of Cr(III), Ru(II) and Ru(III) complexes. Applications- synthesis and catalysis, chemical actinometry and photochromism. Metal-metal multiple bonds.

3.2 Metal complex sensitizers-electron relay, semiconductor supported metal oxide systems, water photolysis, nitrogen fixation and CO_2 reduction.

Module 4: Nanomaterials (18 Hrs)

4.1 General introduction to nanomaterials and emergence of nanotechnology, Moore's law, Graphene (elementary idea only), synthesis and properties of fullerenes and carbon nanotubes, synthesis of nanoparticles of gold, silver, rhodium, palladium and platinum, techniques of synthesis-electroplating and electrophoretic deposition, conversion through chemical reactions and lithography. Thin films-chemical vapour deposition and atomic layer deposition techniques.

4.2 Diversity in nanosystems: self assembled monolayers on gold-growth process and phase transitions. Gas phase clusters- formation, detection and analysis. Quantum dots- preparation, characterization and applications. Nanoshells- types of systems, characterization and application.

4.3 Evolving interfaces of nanotechnology- nanobiology, nanosensors, nanomedicines.

Module 5: Analytical Methods (18 Hrs)

5.1 The basis and procedure of sampling-crushing and grinding, gross sampling. Sampling of solids, liquids, gas, particulate solids, metals and alloys. Preparation of a laboratory sample. Moisture in samples- essential and non essential water, occluded water. Determination of water in samples- direct and indirect methods.

5.2 Decompositions and dissolution-reagents for decomposition and dissolution like HCl, H_2SO_4, HNO_3, $HClO_4$ and HF. Microwave decompositions, combustion methods. Uses of fluxes like Na_2CO_3, Na_2O_2, KNO_3, $K_2S_2O_7$, NaOH, B_2O_3 and lithium meta borate.

5.3 Elimination of interferences from samples by precipitation, electrolytic precipitation, separation by extraction and ion exchange separation.

5.4 Analytical procedures involved in the environmental monitoring of water quality- BOD, COD, DO, nitrite and nitrate, iron, fluoride, soil moisture, salinity, soil colloids, cation and anion exchange capacity. Air pollution monitoring: sampling and collection of air pollutants-SO_2, NO_2, NH_3, O_3, and PMM.

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PG4CHE E02 ORGANIC CHEMISTRY - IV

(ADVANCED ORGANIC CHEMISTRY)

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

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

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

1.2 Molecular receptors: cyclodextrins, crown ethers, cryptands, spherands, tweezers, carcerands, cyclophanes, calixarenes, carbon nanocapsules.

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

1.4 Applications of supramolecular complexes in perfumery and medicine. Targeted drug delivery.

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

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

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

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

2.4 General principles of microwave and ultrasound assisted organic synthesis.

Module 3: Chromatrographic techniques (9 Hrs)

Chromatographic techniques: theory of chromatography, Applications of adsorption, partition, paper, thin layer and column chromatographic methods. LC, HPLC, IEC, GC and GPC. Column matrices. Detectors. Affinity and chiral columns.

Module 4: Stereoselective Transformations (9 Hrs)

4.1 Asymmetric induction-chiral auxiliaries and chiral pool.

4.2 Enantioselective catalytic hydrogenation developed by Noyori and Knowels.

4.3 Asymmetric aldol condensation pioneered by Evans.

4.4 Asymmetric Diels-Alder reactions.

4.5 Asymmetric epoxidation using Jacobsen's catalyst.

Module 5: Chemistry of Natural Products and Biomolecules (27 Hrs)

5.1 Steroids: Classification and nomenclature of steroids. Basic principles of the biosynthesis of steroids. Reactions, structure elucidation, stereochemistry and biosynthesis of cholesterol. Structure and semisynthesis of steroid hormones-testosterone, estrogen. Biomimetic synthesis of progesterone and spatriene.

5.2 Alkaloids: Classification of alkaloids. General methods of structure elucidation of alkaloids. Structure elucidation and synthesis of papaverine, quinine and morphine. Basic principles of the biosynthesis of alkaloids. Biosynthesis of morphine. Biogenesis of alkaloids.

5.3 Terpenoids: Classification of terpenoids. Synthesis of camphor. Basic principles of the biosynthesis of terpenes. Biosynthesis of α-terpineol. Biogenesis of isoprenoids.

5.4 Carbohydrates: Classification of carbohydrates. Basic principles of the biosynthesis of carbohydrates. Biosynthesis of glucose.

5.5 Plant pigments: Anthocyanins and carotenoids. Structure and synthesis of cyanin, flavones, quercetine and β-carotene.

5.6 Lipids: Classification of lipids.

5.7 Vitamins: Classification of vitamins. Structure of vitamins A, B_1, B_2, B_6 and C. Synthesis of vitamins A, B_1, B_2 and C.

5.8 Amino acids, proteins and nucleic acids: Classification. Basic principles of the biosynthesis of proteins and nucleic acids. Biosynthesis of phenyl alanine. Primary, secondary, tertiary and quarternary structure of proteins. Methods for primary structure determination of peptides, proteins and nucleic acids. 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).

5.9 Prostaglandins: Nomenclature. Synthesis of PGE_2 and PGF_2.

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

6.1 Introduction to Drug design:-Drug action, receptor theories, receptor proteins, drug receptor interaction, drug metabolism-different pathways. Combinatorial synthesis and modeling techniques (a brief study).

6.2 Important drugs used in the following classes with mode of action:-. Antibacterial agents (Penicillins, cephalosporins, tetracyclines, chloramphenicol, ciprofloxacin, isoniazid), Antiparasitic agents (Ivermectin), Analgesics (Aspirin), Antiviral agents (Acyclovir, oseltamivir), Anticancer agents (podophyllotoxin, calicheamicin, tamoxifen, paclitaxel), CNS Drugs (Salbutamol, Ephedrine, Phenobarbital), Antisyphilitic agents (Salvarsan), Cholesterol lowering agents (Lovastatin), Immunosuppressants (cyclosporine), Vasodialators (Viagra), Narcotics (Methadone).

6.3 Applications of nanomaterials in medicine.

Module 7: Advances in Polymer Chemistry (9 Hrs)

7.1 Conducting polymers, polymers for NLO applications, 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. Dendrimers as nanocapsules. Applications of dendrimers as organo catalysts. Hyper branched polymers: definition, examples, synthesis and applications.

References

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PG4CHE E03 PHYSICAL CHEMISTRY - IV

(ADVANCED PHYSICAL CHEMISTRY)

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

Module 1: Crystallography **(18 Hrs)**

1.1 Miller indices, point groups (derivation not expected), translational symmetry, glide planes and screw axes, space groups, simple cases like triclinic and monoclinic systems, interplanar spacing and method of determining lattice types, reciprocal lattices, methods of characterizing crystal structure, rotating crystal method, powder X-ray diffraction method, determination of structure of sodium chloride by powder method, comparison of the structures of NaCl and KCl, brief outline of single crystal X-ray diffraction and crystal growth techniques.

1.2 Structure factor: atomic scattering factor, coordinate expression for structure factor, structure by Fourier synthesis.

1.3 Liquid crystals: mesomorphic state, types, examples and applications of liquid crystals. Theories of liquid crystals. Photoconductivity of liquid crystals.

Module 2: Electrochemistry **(18 Hrs)**

2.1 Conductance measurements, results of conductance measurements, ionic mobilities, influence of pressure and temperature on conductance of ions, Walden equations, abnormal ionic conductance.

2.2 Theories of ions in solution, Drude and Nernst's electrostriction model and Born's model, Debye-Huckel theory, Derivation of Debye-Huckel-Onsager equation, validity of DHO equation for aqueous and non aqueous solutions, Debye-Falkenhagen effect, conductance with high potential gradients, activity and activity coefficients in electrolytic solutions, ionic strength, Debye-Huckel limiting law and its various forms, qualitative and quantitative tests of Debye- Huckel limiting equation, deviations from the DHLL. Osmotic coefficient, ion association, fraction of association, dissociation constant, triple ion and conductance minima, equilibria in electrolytes.

2.3 Electrochemical cells, concentration cells and activity coefficient determination, liquid junction potential, evaluation of thermodynamic properties.

Module 3: Electrode Double layer and Polarisation (9 Hrs)

3.1 Electrode double layer, electrode-electrolyte interface, different models of double layer-Helmholtz compact layer model, Guoy-Chapman model, Stern model, theory of multilayer capacity, electrocapillary, Lippmann equation, membrane potential.

3.2 Fuel cells, classification based on working temperature, chemistry of fuel cells, H_2-O_2 fuel cells.

3.3 Polarization - electrolytic polarization, dissolution and decomposition potential, concentration polarization, overvoltage, hydrogen and oxygen overvoltage, theories of overvoltage, Tafel equation and its significance, Butler-Volmer equation for simple electron transfer reactions, transfer coefficient, exchange current density, rate constants.

Module 4: Quantum Statistics (9 Hrs)

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

4.2 Heat capacity of solids- Dulong and Petit's law, the vibrational properties of solids, Einsteins theory- derivation and its limitations. Debye theory – derivation and its limitations.

Module 5: Electroanalytical Techniques (18 Hrs)

5.1 Voltametry and polarography: Voltametry-cyclic voltametry, ion-selective electrodes, anodic stripping voltametry. Polarography- decomposition potential, residual current, migration current, supporting electrolyte, diffusion current, polarogram, half wave potential, limiting current density, polarograph, explanation of polarographic waves, the dropping mercury electrode, advantages and limitations of DME, applications of polarography, quantitative analysis- pilot ion procedure, standard addition method, qualitative analysis-determination of half wave potential of an ion, advantages of polarography.

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

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

Module 6: Diffraction Methods, Atomic Spectroscopic Techniques and Fluorescence Spectroscopy (18 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.

6.5 Fluorescence sensing, mechanism of sensing, sensing techniques based on collisional quenching, energy transfer and electron transfer, examples of pH sensors. Novel fluorophores: long life time metal-ligand complexes.

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[1] L.V. Azaroff, Introduction to Solids, McGraw Hill, 1984.

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PG4CHE E04 - POLYMER CHEMISTRY

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

Module 1: Introduction to Polymer Science (9 Hrs)

1.1 History of macromolecular science: monomers, functionality, degree of polymerization, classification of polymers based on origin, structure, backbone, branching, action of heat, ultimate form and use, tacticity and crystalline behaviour.

1.2 Primary bonds-molecular forces in polymers: dipole forces, induction forces, dispersion forces and H bond, dependence of physical properties on intermolecular forces. Polymer molecular weight-different averages, polydispersity index, molecular weight distribution curve, polymer fractionation. Methods for molecular weight determination: end group analysis, colligative property measurements, ultracentrifugation, vapour phase osmometry, viscometry, GPC, light scattering method. Monomers and structure of common polymers like PE, PP, PVC, PVAc, PVA, PMMA, PEMA, poly lactic acid, PET, PBT, PS, PTFE, PEI, nylon 6, nylon 66, nylon 612, Kevlar, PEEK, PES, PC, ABS, PAN, PEO, PPO, PEG, SAN, PCL, PLA, PHB, DGEBA, MF, UF, AF, PF, PU, NR, SBR, NBR, PB, butyl rubber, polychloroprene and thiokol rubber.

Module 2: Fundamentals of Polymerization (18 Hrs)

2.1 Addition polymerization, free radical addition polymerization, mechanism and kinetics of vinyl polymerization, kinetics of free radical addition polymerization, effect of temperature, pressure, enthalpies, entropies, free energies and activation energies on polymerization.

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

2.3 Mechanism of coordination polymerization, Ziegler-Natta polymerization, ring opening polymerization, mechanism of polymerization of cyclic amides.

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

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

2.6 Controlled polymerization methods, nitroxide mediated polymerization, Ring Opening polymerization (ROP), Atom Transfer Radical Polymerization (ATRP), Reversible Addition Fragmentation Termination (RAFT).

Module 3: Properties of Polymers (18 Hrs)

3.1 Structure property relationship in polymers, transitions in polymers, first order and second order transitions in polymers, relationship between Tg and Tm, molecular motion and transitions, Boyer-Beamem rule, factors affecting glass transition temperature.

3.2 Rheological properties of polymers, Newtonian fluids, non-Newtonian fluids, pseudoplastic, thixotropy, St. Venant body, dialatant, complex rheological fluids, rheopectic fluids, time dependent fluids, time independent fluids, power law, Weissenberg effect, laminar flow, turbulent flow, die swell, shark skin, viscous flow.

3.3 Viscoelastic properties of polymers, viscoelasticity, Hooke's law, Newton's equation, viscoelastic models-time temperature equivalence, WLF equation, Boltzmann superposition principle, linear stress - strain relations for other types of deformation-creep, stress relaxation. Temperature dependence of viscosity. Transport in polymers - diffusion, liquid and gas transport, Fick's law, theories of diffusion.

Module 4: Stereochemistry and Conformation of Polymers (9 Hrs)

Stereoregular polymers, constitutional isomerism, positional isomerism and branching, optical isomerism, geometric isomerism, substitutional isomerism, configuration of polymer chains, infrared, Raman and NMR characterization, polymer conformation, chain end to end distance, random walks and random flights, self-avoiding walks.

Module 5: Morphology and Order in Crystalline Polymers (9 Hrs)

5.1 Polymer morphology, common polymer morphologies, structural requirements for crystallinity, degree of crystallinity, crystallisability- mechanism of crystallization, polymer single crystals, lamellar structure of polymers, fringed micelle concept, folded chain model, adjacent re-entry model, switchboard model.

5.2 Structure of polymers crystallised from melt, spherulitic morphology, mechanism of spherulite formation, theories of crystallisation kinetics, Avrami equation, Hoffman's nucleation theory, the entropic barrier theory, strain induced morphology, cold drawing, morphology changes during orientation, application of XRD, SEM and DSC in determining the crystallinity of polymers.

Module 6: Advances in Polymers (9 Hrs)

6.1 Specialty polymers, conducting polymers, high temperature polymers, flame resistant polymers, biopolymers and biomaterials, polymers in medicine, polymers for dental applications.

6.2 Carbon fibres. Synthesis, characterization and applications of carbon nanofibres.

Module 7: Dendrimers and Dendritic Polymers (18 Hrs)

7.1 Basic concepts and terminology: Dendrons, star shaped and star bust polymers, dendrimer formation and generations, various types of dendrimers.

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

7.3 Characterisation of dendrimers: GPC, osmosis, TG, DSC, magnetic resonance spectroscopy (^{1}H and ^{13}C NMR), mass spectral studies (MALDI and TOF).

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

References

1. V.R. Gowariker, N.V. Viswanathan, J. Sreedhar, Polymer Science, New Age International, 2003.
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12. H.R. Allock, F. W. Lampe, Contemporary Polymer Chemistry, Pearson/Prentice Hall, 2003.

PG4CHE E05 ANALYTICAL CHEMISTRY

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

Module 1: Instrumental Methods (36 Hrs)

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

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

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

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

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

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

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

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

Module 2: Sampling (18 Hrs)

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

2.2 Decomposition and dissolution, source of error, reagents for decomposition and dissolution like HCl, H_2SO_4, HNO_3, $HClO_4$, HF, microwave decompositions, combustion methods, use of fluxes like Na_2CO_3, Na_2O_2, KNO_3, NaOH, $K_2S_2O_7$, B_2O_3 and lithium metaborate. Elimination of interference from samples - separation by precipitation, electrolytic precipitation, extraction and ion exchange. Distribution ratio and completeness of multiple extractions. Types of extraction procedures.

Module 3: Applied Analysis (9 Hrs)

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

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

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

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

Module 4: Capillary Electrophoresis and Capillary Electro Chromatography (9 Hrs)

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

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

Module5: Process instrumentation (9 Hrs)

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

Module 6: Aquatic Resources (9 Hrs)

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

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

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

References

[1] J.M. Mermet, M. Otto, R. Kellner, Analytical Chemistry, Wiley-VCH, 2004.

[2] D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College Pub., 2007.

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SEMESTERS 3 AND 4

PG4CHE P04– INORGANIC CHEMISTRY PRACTICAL – 2

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

PART I

Estimation of simple binary mixtures (like Cu-Ni, Cu-Zn, Fe-Cr, Fe-Cu, Fe-Ni, Pb-Ca) of metallic ions in solution by volumetric and gravimetric methods.

PART II

Analysis of one of the alloys of brass, bronze and solder. Analysis of one of the ores from hematite, chromite, dolomite, monazite, illmenite.

References

[1] A.I. Vogel, A Text Book of Quantitative Inorganic Analysis, Longman, 1966.

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PG4CHE P05 ORGANIC CHEMISTRY PRACTICAL-2

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

PART I

A. Volumetric estimation of 1) Aniline 2) Phenol 3) glucose 4) Iodine value and saponification value of oil

B. Spectrophotometric/colorimetric estimation of 1) Aniline 2) Glucose 3) Cholesterol 4) ascorbic acid 5) Streptomycin 6) Aspirin.

PART II

Preparation of compounds by two stages.

1) Acetanilide – p-nitroacetanilide – p-nitroaniline
2) Methyl benzoate – m-nitromethylbenzoate – m-nitrobenzoic acid
3) Acetanilide – p-bromoacetanilide – p-bromoaniline
4) Phenol – salicylaldehyde – coumarin
5) Benzophenone – benzophenone oxime – benzanilide
6) Aniline – 2,4,6-tribromoaniline – 1,3,5-tribromoaniline
7) Benzaldehyde-benzoin-benzilic acid
8) Aniline-sulphanilic acid-methylorange
9) O-Toluidine-o-methyl acetanilide-N-acetyl anthranilic acid
10) Aniline-acetanilide-p-nitroacetanilide

PART III

Enzyme/coenzyme catalyzed reactions.

PART IV

Preparation Involving Green Alternatives of Chemical Methods.

PART V

Microwave assisted Organic Synthesis.

PART VI

Prediction of FTIR, UV-Visible, ^{1}H and ^{13}C NMR spectra of the substrates and products at each stage of the products synthesized by the above methods.

PART VII – Viva - voce

References

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[2] A.I. Vogel, Elementary Practical Organic Chemistry, Longman, 1958.

[3] F.G. Mann and B.C Saunders, Practical Organic Chemistry, 4th Edn., Pearson Education India, 2009.

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PG4CHE P06 PHYSICAL CHEMISTRY PRACTICAL-2

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

I Chemical Kinetics

1. Determination of the rate constant of the acid / alkaline hydrolysis of ester.
2. Determination of Arrhenius parameters.
3. Kinetics of reaction between $K_2S_2O_8$ and KI
4. Influence of ionic strength on the rate constant of the reaction between $K_2S_2O_8$ and KI
5. Iodination of acetone in acid medium.

II Polarimetry

1. Kinetics of the inversion of sucrose in presence of HCl.
2. Determination of the concentration of a sugar solution.
3. Determination of the concentration of HCl.
4. Determination of the relative strength of acids.

III Refractometry

1. Identification of pure organic liquids and oils.
2. Determination of molar refractions of pure liquids.
3. Determination of concentration of solutions (KCl-water, glycerol-water).
4. Determination of molar refraction of solids.
5. Study of complex formation between potassium iodide and mercuric iodide system.

IV Viscosity

1. Determination of viscosity of pure liquids.
2. Verification of Kendall's equation.
3. Determination of the composition of binary liquid mixtures (alcohol-water, benzene-nitrobenzene).
4. Determination of the molecular weight of a polymer (polystyrene in toluene).

V Conductivity measurements

1. Verification of Onsager equation.
2. Determination of the degree of ionization of weak electrolytes.
3. Determination of pKa values of organic acids.
4. Determination of solubility of sparingly soluble salts.
5. Titration of a mixture of acids against a strong base.
6. Titration of a dibasic acid against a strong base.

VI Potentiometry

1. Determination of single electrode potentials (Cu and Zn).
2. Application of Henderson equation.
3. Titrations.
4. Determination of end point of a titration using Gran Plot.
5. Determination of the concentration of a mixture of Cl^- and I^- ions.

References

[1] J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.

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

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M.Sc. ANALYTICAL CHEMISTRY

M.Sc. ANALYTICAL CHEMISTRY

	Code	Course	Hours/ week	Total Hours	Credit	Marks		
						Internal	External	Total
Semester 1	PG1ANL C01	Inorganic Chemistry-I (Coordination & Nuclear Chemistry)	4	72	4	20	80	100
	PG1ANL C02	Organic Chemistry-I (Structure, Reactivity & Stereochemistry)	4	72	4	20	80	100
	PG1ANL C03	Theoretical Chemistry-I (Quantum Chemistry and Group Theory)	4	72	4	20	80	100
	PG1ANL C04	Physical chemistry- I (Kinetic Theory, Thermodynamics and Statistical Thermodynamics)	3	54	3	20	80	100
	PG2ANL P01	Inorganic Chemistry Practical–1	3	54	Evaluation at the end of second semester			
	PG2ANL P02	Organic Chemistry Practical-1	3	54				
	PG2ANL P03	Physical Chemistry Practical -1	4	72				
		Total	**25**	**450**	**15**			
Semester 2	PG2ANL C05	Inorganic Chemistry-II (Bioinorganic & Organometallic Chemistry)	4	72	4	20	80	100
	PG2ANL C06	Organic Chemistry- II (Reaction Mechanism)	4	72	4	20	80	100
	PG2ANL C07	Theoretical Chemistry – II (Chemical Bonding and Computational Chemistry)	4	72	4	20	80	100
	PG2ANL C08	Physical chemistry- II (Molecular Spectroscopy)	3	54	3	20	80	100
	PG2ANL P01	Inorganic Chemistry Practical–1	3	54	3	20	80	100
	PG2ANL P02	Organic Chemistry Practical-1	3	54	3	20	80	100
	PG2ANL P03	Physical Chemistry Practical -1	4	72	4	20	80	100
		Total	**25**	**450**	**25**			

Semester 3	PG3ANL C09	Inorganic chemistry-III (Solid State Chemistry)	4	72	4	20	80	100
	PG3ANL C10	Organic chemistry- III (Organic Syntheses)	4	72	4	20	80	100
	PG3ANL C11	Physical chemistry- III (Chemical Kinetics, Surface Chemistry and Photochemistry)	4	72	4	20	80	100
	PG3ANL C12	Spectroscopic Methods in Chemistry	3	54	3	20	80	100
	PG4ANL P04	Inorganic Chemistry Practical–2	3	54	Evaluation at the end of fourth semester			
	PG4ANL P05	Organic Chemistry Practical-2	3	54				
	PG4ANL P06	Instrumental Analysis Practical	4	72				
		Total	**25**	**450**	**15**			
Semester 4	PG4ANL E01	Elective –I Analytical Procedures	5	90	4	20	80	100
	PG4ANL E02	Elective –II Instrumental Methods of Analysis	5	90	4	20	80	100
	PG4ANL E03	Elective –III Modern Analytical Techniques And Green chemistry	5	90	4	20	80	100
	PG4ANL E04	Elective –IV Polymer Chemistry	5	90	4	20	80	100
	PG4ANL E05	Elective –V Applied Analysis and Aquatic Resources	5	90	4	20	80	100
	PG4ANL P04	Inorganic Chemistry Practical–2	3	54	3	20	80	100
	PG4ANL P05	Organic Chemistry Practical-2	3	54	3	20	80	100
	PG4ANL P06	Instrumental Analysis Practical	4	72	3	20	80	100
	PG4ANL D01	Project			2	20	80	100
	PG4ANL V01	Viva			2	20	80	100
		Total	**25**	**450**	**25**			
Grand Total					**80**			

SEMESTER 1

PG1ANL C01 INORGANIC CHEMISTRY – I

(COORDINATION & NUCLEAR CHEMISTRY)

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

Module 1: Coordination Chemistry- Structural Aspects and Bonding (18 Hrs)

1.1 Classification of complexes based on coordination numbers and possible geometries. σ and π bonding ligands such as CO, NO, CN^-, R_3P and Ar_3P.

1.2 Splitting of *d* orbitals in octahedral, tetrahedral, square planar, square pyramidal and trigonal 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 with and without π-bonding, experimental evidences for π-bonding

Module 2: Kinetics and Mechanism of Reactions in Metal Complexes (18 Hrs)

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

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

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

Module 3: Organometallic Compounds- Synthesis, Structure and Bonding (18 Hrs)

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

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

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

Module 4: Electron deficient compounds (9 Hrs)

Electron deficient compounds – synthesis, reactions, structure and bonding. Boron hydrides, styx numbers, Boron cluster compounds.

Wade's rule, Hydroborate anions, Organoboranes and hydroboration, Polyhedral anions, Carboranes, Metalloboranes, Borazines and Borides.

Module 5: Nuclear Chemistry (9 Hrs)

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

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

5.3 Analytical applications of radioisotopes- radiometric titrations, kinetics of exchange reactions, measurement of physical constants including diffusion constants, neutron activation analysis, prompt gamma neutron activation analysis and neutron absorptiometry.

5.4 Applications of radio isotopes in industry, medicine, autoradiography, radiopharmacology, radiation safety precaution, nuclear waste disposal.

5.5 Radiation chemistry of water and aqueous solutions- Fricke solution, Ceric ammonium solution. Measurement of radiation doses. Relevance of radiation chemistry in biology, organic compounds and radiation polymerization.

References

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PG1ANL C02 ORGANIC CHEMISTRY - I

(STRUCTURE, REACTIVITY & STEREOCHEMISTRY)

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

Module 1: MO Theory and Aromaticity (9 Hrs)

1.1 Review of basic concepts in organic chemistry: bonding, hybridization, MO picture (allyl system, 1,3-butadiene and benzene), inductive effect, electromeric effect, resonance effect, hyperconjugation, steric effect. Bonding weaker than covalent bonds.

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

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

Module 2: Investigation of Organic Reaction Mechanisms (9 Hrs)

Energy profiles, Methods of determining reaction mechanisms, Kinetic and thermodynamic control of reactions. The Hammond postulate. Principle of microscopic reversibility. Marcus theory. The Hammett equation and its applications. Taft equation. Linear free energy relationships. Solvent polarity and parameters. Y, Z and E parameters and their applications. Primary and secondary kinetic isotope effects. Salt effects and special salt effects in SN reactions. Solvent effect. Bulk and specific solvent effects. Introduction to carbon acids - pKa of weak acids, kinetic and thermodynamic acidity. Phase transfer catalysis and its applications. Steric effects. HSAB principle and its applications in organic reactions.

Module 3: Review of Organic Reaction Mechanisms (18 Hrs)

3.1 Review of organic reaction mechanisms with special reference to nucleophilic and electrophilic substitution at aliphatic carbon (S_N1, S_N2, S_Ni, S_E1, S_E2, addition-elimination and elimination-addition sequences), elimination (E1 and E2). Elimination vs substitution.

3.2 A comprehensive study on the effect of substrate, reagent, leaving group, solvent and neighbouring group on nucleophilic substitution (S_N2 and S_N1) and elimination (E1 and E2) reactions.

3.3 Addition reactions (regioselectivity- Markovnikov's addition- carbocation mechanism, anti-Markovnikov's addition- radical mechanism).

3.4 Mechanism of electrophilic and nucleophilic aromatic substitution reactions with examples. Arenium ion intermediates. S_N1, S_NAr, $S_{RN}1$ and Benzyne mechanisms.

3.5 Catalysis by acids, bases and nucleophiles with examples from acetal, cyanhydrin and ester formation and hydrolysis reactions- $A_{AC}2$, $A_{AC}1$, $A_{AL}1$, $B_{AC}2$ and $B_{AL}1$ mechanisms.

Module 4: Stereochemistry of Organic Compounds (18 Hrs)

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

4.2 Stereoisomerism: Definition based on symmetry and energy criteria, configurational and conformational stereoisomers.

4.3 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 C_n, molecules with more than one center of chirality, definition of diastereoisomers, constitutionally symmetrical and unsymmetrical chiral molecules, erythro and threo nomenclature.

4.4 Axial, planar and helical chirality with examples, stereochemistry and absolute configuration of allenes, biphenyls, binaphthyls, ansa and cyclophanic compounds, spiranes, exocyclic alkylidene cycloalkanes.

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

4.6 Geometrical isomerism: Nomenclature, E-Z notation, methods of determination of geometrical isomers. Interconversion of geometrical isomers.

Module 5: Conformational Analysis (18 Hrs)

5.1 Conformational descriptors- factors affecting conformational stability of molecules. Conformational analysis of acyclic and cyclic systems: substituted ethanes, cyclohexane and its derivatives, decalins, adamantane, congressane, sucrose and lactose. Fused and bridged bicyclic systems.

5.2 Conformation and reactivity of elimination (dehalogenation, dehydrohalogenation, semipinacolic deamination and pyrolytic elimination- Saytzeff and Hofmann eliminations), substitution and oxidation of 2° alcohols. Chemical consequence of conformational equilibrium - Curtin Hammett principle. Chiral drugs.

References

[1] R. Bruckner, Advanced Organic Chemistry: Reaction Mechanisms, Academic Press, 2002.

[2] I. Fleming, Frontier Orbitals and Organic Chemical Reactions, Wiley, 1976.

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PG1ANL C03 THEORETICAL CHEMISTRY – I

(QUANTUM CHEMISTRY AND GROUP THEORY)

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

Module 1: Formulation of Quantum Chemistry (18 Hrs)

1.1 Mathematical Concepts (5 Hrs)

Co-ordinate systems: Cartesian, Cylindrical polar and Spherical polar coordinates and their relationships. Complex numbers: definition, Complex conjugate, absolute value of a complex number, complex functions. Operator algebra: linear and nonlinear operators, Hermitian operators, del and del-squared operators. Eigen function and eigen values of an operator, Eigen value equation, Eigen functions of Commuting operators. Well behaved functions, Normalized and Orthogonal functions.

1.2 Evolution of Quantum Mechanics (5 Hrs)

Failure of classical mechanics: The black body radiation, Compton effect, photoelectric effect, atomic spectra. Need of quantum mechanics. Concept of matter wave, de Broglie relation and its experimental proof, Uncertainty principle and its consequences. Wave function and Born interpretation, Schrödinger's wave mechanics, Deduction of Schrodinger equation from classical wave equation.

1.3 Postulates of Quantum Mechanics (4 Hrs)

Detailed discussion of postulates: State function postulate. Operator postulate. Eigen value postulate. Expectation value postulate. Postulate of time dependent Schrodinger equation of motion, Conservative system and time-independent Schrodinger equation.

1.4 Quantum Mechanics of Translational Motion (4 Hrs)

Particle in one-dimension with infinite potential walls, particle in a three dimensional box- separation of variables- rectangular box and cubic box, degeneracy. Introduction to tunnelling with experimental evidence.

Module 2: Applications of Quantum Chemistry (18 Hrs)

2.1 Quantum Mechanics of Hydrogen-like Atoms (5 Hrs)

Potential energy of hydrogen-like systems. The wave equation in spherical polar

coordinates: separation of variables- R, Θ and Φ equations and their solutions, wave functions and energies of hydrogen-like atoms. Orbitals- radial functions, radial distribution functions, angular functions and their plots.

2.2 Quantum Mechanics of Vibrational Motion (5 Hrs)

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. Rodrigue's formula, Three dimensional harmonic oscillator.

2.3 Quantum Mechanics of Rotational Motion (5 Hrs)

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 Φ equation and its solution, wave functions in the real form. Non-planar rigid rotor (or particle on a sphere)- separation of variables, the Φ and the Θ equations and their solutions, Legendre and associated Legendre equations, Legendre and associated Legendre polynomials. Spherical harmonics (imaginary and real forms)- polar diagrams of spherical harmonics.

2.4 Orbital and Spin angular momentum (3 Hrs)

Quantisation of angular momentum, quantum mechanical operators corresponding to angular momenta, (L_x, L_y, L_z and L^2). Commutation relations between these operators. Spherical harmonics as eigen functions of angular momentum operators L_z and L^2. Space quantization. The postulate of spin by Uhlenbeck and Goudsmith, discovery of spin- Stern Gerlach experiment. Spin orbitals- construction of spin orbitals from orbital and spin functions.

Module 3: Molecular Symmetry and Mathematical group (18 Hrs)

3.1 Symmetry elements and symmetry operations. Conditions for a set of elements to form a group, sub groups, abelian and cyclic groups, Point groups. Multiplication of operations. Group multiplication table of C_{2v}, C_{2h} and C_{3v} groups (H_2O, Trans N_2F_2 and NH_3 as examples). Similarity transformation and classes in a group.

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

3.3 Reducible and Irreducible representations (IR). Reduction formula, reduction of reducible representation to IRs.

Module 4: Applications of Group Theory (18 Hrs)

4.1 The Great Orthogonality theorem. Rules derived from GOT (proof not required). Setting up of character table of C_{2v}, C_{3v}, C_{2h}, C_{4v} and C_3 groups. Direct product representations.

4.2 Applications in quantum mechanics, transition moment integral, vanishing of integrals. Jahn – Teller effect, Woodward – Hoffmann rules.

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

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

References

[1] I.N. Levine, Quantum Chemistry, 6th Edn., Pearson Education Inc., 2009.

[2] P.W. Atkins, R.S. Friedman, Molecular Quantum Mechanics, 4th Edn., Oxford University Press, 2005.

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PG1ANL C04 - PHYSICAL CHEMISTRY - 1

(KINETIC THEORY, THERMODYNAMICS AND STATISTICAL THERMODYNAMICS)

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

Module 1: Kinetic theory (9 Hrs)

Kinetic theory of gases, 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, transport properties of gases. Viscosity, thermal conductivity and diffusion. Determination of viscosity of gases. Influence of temperature and pressure on transport properties.

Module 2: Classical Thermodynamics (18 Hrs)

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

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

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

2.4 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.

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

2.6 Chemical affinity and thermodynamic functions, effect of temperature and pressure on chemical equilibrium- van't Hoff reaction isochore and isotherm.

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

2.8 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, and three pairs of partially miscible liquids.

Module 3: Irreversible Thermodynamics and Bioenergetics (9 Hrs)

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

Module 4: Statistical Thermodynamics (18 Hrs)

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

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

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SEMESTER II

PG2ANL C05 INORGANIC CHEMISTRY- II

(BIOINORGANIC & ORGANOMETALLIC CHEMISTRY)

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

Module 1: Acids, Bases and Non-aqueous solvents (9 Hrs)

1.1 Acid base concept in non-aqueous media-HSAB concept, solvent effect, linear free energy relationship- mechanism and method of determination.

1.2 Reaction in non-aqueous solvents. Ammonia- solution of metals in liquid ammonia. Protonic solvents: anhydrous sulphuric acid, hydrogen halide. Aprotic solvents: non-polar solvents, non-ionizable polar solvents. Polar solvents undergoing autoionization. Liquid halogen, Inter halogen compounds, oxy halides, dinitrogen tetroxide, sulphur dioxide.

Module 2: Bioinorganic Compounds (18 Hrs)

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

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

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

Module 3: Spectral and Magnetic Properties of Metal Complexes (18 Hrs)

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

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

3.3 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.

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

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

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

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

Module 5: Stereochemistry of Coordination Compounds (9 Hrs)

5.1 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.

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

Module 6: Reactions of Organometallic Compounds (9 Hrs)

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

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

6.3 Rearrangement reactions, redistribution reactions, fluxional isomerism.

References

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

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

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PG2ANL C06 ORGANIC CHEMISTRY - II
(REACTION MECHANISM)

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

Module 1: Chemistry of Carbocations (9 Hrs)

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

1.2 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, Demjanov rearrangement. Oxymercuration, halolactonisation.

Module 2: Chemistry of Carbanions (18 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, Kinetic and thermodynamic enolates- Lithium and boron enolates in Michael and aldol reactions, alkylation and acylation of enolates. Chemistry of enamines, Stork-Enamine reaction.

2.2 Nucleophilic additions to carbonyls groups. Reactions involving carbanions-mechanisms of Claisen, Dieckmann, Knoevenagel, Stobbe, Darzen and acyloin condensations, Shapiro reaction and Julia elimination. Favorskii rearrangement.

2.3 Reactions of carbonyl compounds: oxidation, reduction (Clemmensen and Wolff-Kishner), addition reactions (addition of cyanide, ammonia, alcohol), Aldol condensation, Cannizzaro reaction, addition of Grignard reagent.

2.4 Structure and reactions of α, β- unsaturated carbonyl compounds involving electrophilic and nucleophilic addition- Michael addition, Mannich reaction, Robinson annulation.

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

Module 3: Carbenes, Carbenoids, Nitrenes and Arynes (9 Hrs)

3.1 Generation, structure and reactions of carbenes. Rearrangement reactions of carbenes: Wolff rearrangement, generation and reactions of ylids by carbenoid decomposition.

3.2 Structure, generation and reactions of nitrenes. Hoffmann, Curtius, Lossen, Schmidt and Beckmann rearrangement reactions.

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

Module 4: Radical Reactions (9 Hrs)

4.1 Generation and detection 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. Autoxidation.

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

Module 5: Concerted reactions (18 Hrs)

5.1 Symmetry properties of molecular orbitals of ethylene and conjugated systems with three or more atoms, Woodward – Hoffmann rule, Conservation of orbital symmetry and stereo chemical courses.

5.2 Pericyclic reactions like Electrocyclic (butadiene-cyclobutene and hexatriene-cyclohexadiene interconversions), Cycloadditions (2+2) & (4+2), Sigmatropic (1,3), (1,5) and (3,3), Cheletropic including Cheletropic eliminations and Ene reaction with stereo chemical aspects.

5.3 Diels- Alder reactions with stereochemical aspects.

5.4 Analysis of Pericyclic Reactions. (i) FMO method (ii) Orbital- correlation method and (iii) PMO method.

5.2 Highlighting pericyclic reactions in organic synthesis such as Claisen, Cope, Mislow-Evans, Wittig and Sommelet-Hauser rearrangements. dipolar cycloaddition (introductory). Unimolecular pyrolytic elimination reactions, decomposition of cyclic azo compounds, β-eliminations involving cyclic transition states such as N-oxides, acetates and xanthates.

Module 6: Organic Photochemistry (9 Hrs)

6.1 Photochemical processes. Energy transfer. Jablonski diagram, sensitization and quenching. Singlet and triplet states and their reactivity.

6.2 Photoreactions of carbonyl compounds, enes, dienes and arenes. Norrish reactions of acyclic ketones. Patterno-Buchi, Barton, Photo-Fries and Di-л methane rearrangements. Photoreactions of Vitamin D. Photosynthesis and photochemistry of vision. Singlet oxygen generation and their reactions.

References

[1] R. Bruckner, Advanced Organic Chemistry: Reaction Mechanism, Academic Press, 2002.

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[14] Jagadamba Singh, Jaya Singh, Photochemistry and Pericyclic Reactions, 3rd Edn., New Age International Publ. Ltd.

PG2ANL C07 THEORETICAL CHEMISTRY - II

(CHEMICAL BONDING AND COMPUTATIONAL CHEMISTRY)

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

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

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

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

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

Module 2: Chemical Bonding (18 Hrs)

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

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

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

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

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

Module 4: Computational Chemistry (18 Hrs)

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

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

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

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

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

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

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

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

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

Module 5: Computational Chemistry Calculations (9 Hrs)

5.1 Molecular geometry input-cartesian coordinates and internal coordinates, Z-matrix. Z-matrix of: single atom, diatomic molecule, non-linear triatomic molecule, linear triatomic molecule, polyatomic molecules like ammonia, methane, ethane and butane. General format of GAMESS/Firefly input file. GAMESS/Firefly key word for: basis set selection, method selection, charge, multiplicity, single point energy calculation, geometry optimization, constrained optimization and frequency calculation.

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

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

References

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Softwares

Molecular Mechanics:

01. **Arguslab** available from www.arguslab.com/
02. **Tinker** available from www.dasher.wustl.edu/ffe/

Ab initio, semiempirical and dft:

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

Graphical User Interface (GUI):

01. **Gabedit** available from http://gabedit.sourceforge.net/
02. **wxMacMolPlt** available from http://www.scl.ameslab.gov/MacMolPlt/
03. **Avogadro** from http://avogadro.openmolecules.net/wiki/Get_Avogadro

PG2ANL C08 PHYSICAL CHEMISTRY - II

(MOLECULAR SPECTROSCOPY)

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

Module 1: Microwave and Infrared Spectroscopy (18 Hrs)

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

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

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

Module 2: Electronic, Mossbauer and Raman spectroscopy (18 Hrs)

2.1 Electronic spectroscopy: Term symbols of diatomic molecules, electronic spectra of diatomic molecules, selection rules, vibrational coarse structure and rotational fine structure of electronic spectrum, Franck-Condon principle, predissociation, calculation of heat of dissociation, Birge and Sponer method, electronic spectra of polyatomic molecules, spectra of transitions localized in a bond or group, free electron model.

Different types of lasers- solid state lasers, continuous wave lasers, gas lasers and chemical laser, frequency doubling, applications of lasers, introduction to UV and X-ray photoelectron spectroscopy.

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

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

Module 3: Resonance Spectroscopy (18 Hrs)

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

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

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

3.4 An elementary study of NQR spectroscopy.

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

[4] R.S. Drago, Physical Methods in Inorganic Chemistry, Van Nonstrand Reinhold, 1965.

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SEMESTERS 1 ANDS 2

PG2ANL P01 INORGANIC CHEMISTRY PRACTICAL – 1

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

PART I

Separation and identification of four metal ions of which two are rare/ less familiar such as Tl, W, V, Se, Te, Ti, Ce, Th, Zr, U, Mo and Li and common cations - 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+}, Co^{2+}, Ni^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}, Mg^{2+}, Li^{+}, Na^{+}, K^{+}, NH_4^{+} (interfering acid radicals are not present). Confirmation by spot test (Minimum **8** mixtures are to be recorded).

PART II

1. Argentometric estimation of chlorides
2. Cerimetry – Fe(II) and nitrate
3. Potassium iodate – iodide estimation of Sn(II)

PART III

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

PART IV

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

1. Tris (thiourea) copper (I) complex
2. Potassium tris (oxalate) aluminate (III)
3. Tetrammine copper (II) sulphate
4. Mercury tetra thiocyanato cobaltate (III)

References

[1] A.I. Vogel, A Text Book of Qualitative Inorganic Analysis Including Elementary Instrumental Analysis, 3rd Edn., ELBS.

[2] G. Svelha, Text Book of Vogel's Macro and Semi-micro Inorganic Analysis, revised, Orient Longman.

[3] V.V. Ramanujam, Inorganic Semi micro Qualitative Analysis, The National Publishing Co., Chennai.

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

PG2ANL P02 ORGANIC CHEMISTRY PRACTICAL - 1

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

PART I

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

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

PART II

A. Separation of organic binary mixtures:- 1. Quantitative separation of a mixture oftwo components by solvent extraction 2. Purification of the separated samples by distilling and crystallization. 3. Determination of physical constants of separated and purified samples (No need of bifunctional compounds).

B. Separation of organic mixtures by TLC and calculation of R_f values.

C. Separation/purification of organic mixtures by column chromatography.

PART III

Drawing the structures of organic molecules and reaction schemes and mechanisms by ChemDraw, SymyxDraw and Chemsketch.

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

PART IV- Viva voce

References

[1] A.I. Vogel, A Textbook of Practical Organic Chemistry, Longman, 1974.

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PG2ANL P03 PHYSICAL CHEMISTRY PRACTICAL - 1

Credit: 4 **Contact Lab Hours: 72+72 =144**

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

Part A

I. Adsorption

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

II. Phase diagrams

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

III. Distribution law

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

IV. Surface tension

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

Part B

Computational Chemistry Experiments

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

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

References

[1] J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.

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

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

[4] GAMESS documentation available from: http://www.msg.ameslab.gov/gamess/documentation.html.

SEMESTER 3

PG3ANL C09 INORGANIC CHEMISTRY –III

(SOLID STATE CHEMISTRY)

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

Module 1: Solid State Chemistry **(18 Hrs)**

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

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

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

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

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

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

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

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

Module 3: Inorganic Chains and Rings (18 Hrs)

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

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

Module 4: Organometallic Polymers (9 Hrs)

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

Module 5: Chemistry of Materials (9 Hrs)

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

References

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PG3ANL C10 – ORGANIC CHEMISTRY – III

(ORGANIC SYNTHESES)

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

Module 1: Retrosynthetic Analysis **(9 Hrs)**

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

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

Module 2: Organometallics **(9 Hrs)**

Preparation and applications in organic synthesis of (i) Organo lithium compounds and addition to −C=O, −COOH and –$CONR_2$ (ii) Lithium dialkylcuprates (Gilman reagent) and reaction with alkyl halides, aryl halides and enones (iii) Alkynyl Cu(I) reagents and Glaser coupling (iv) Dialkyl cadmium compounds and (v) Benzenetricarbonyl chromium and reaction with carbanions.

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

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

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

Module 4: Modern Synthetic Methods and Reagents (18 Hrs)

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

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

Module 5: Construction of Carbocyclic and Heterocyclic Ring System (9 Hrs)

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

5.2 Formation of heterocyclic rings: 5- and 6-membered and condensed ring heterocyclic compounds with one or more than one hetero atom like N, S or O - pyrrole, furan, thiophene, pyridine, imidazole, thiazole, oxazole, pyrimidines, purines, quinoline and isoquinoline.

Module 6: Protecting Group Chemistry (9 Hrs)

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

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

6.3 Role of trimethyl silyl group in organic synthesis.

References

[1] M.B. Smith, Organic Synthesis, 3rd Edn., Wavefunction Inc., 2010.

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PG3ANL C11 – PHYSICAL CHEMISTRY – III

(CHEMICAL KINETICS, SURFACE CHEMISTRY AND PHOTOCHEMISTRY)

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

Module 1: Chemical Kinetics **(18 Hrs)**

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

1.2 Lindemann-Hinshelwood mechanism, qualitative idea of RRKM theory, chain reactions: free radical and chain reactions, steady state treatment, Kinetics of H_2-Cl_2 and H_2-Br_2 reactions, Rice-Herzfeld mechanism, branching chains H_2-O_2, Semonov-Hinshelwood mechanism of explosive reactions, mechanisms of step- growth, ionic and addition polymerization, kinetics of anionic and cationic polymerization.

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

1.4 Reactions in solution: factors determining reaction rates in solutions, effect of dielectric constant and ionic strength, cage effect, Bronsted-Bjerrum equation, primary and secondary kinetic salt effect, influence of solvent on reaction rates, significance of volume of activation, linear free energy relationship, kinetic isotope effect.

Module 2: Surface Chemistry **(18 Hrs)**

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

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

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

Module 3: Catalysis (9 Hrs)

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

3.2 Enzyme catalysis and its mechanism, Michaelis-Menton equation, effect of pH and temperature on enzyme catalysis.

3.3 Mechanisms of heterogeneous catalysis: unimolecular and bimolecular surface reactions, mechanisms of catalyzed reactions like ammonia synthesis, Fischer-Tropsch reactions, hydrogenation of ethylene and catalytic cracking of hydrocarbons and related reactions.

Module 4: Colloids and Macromolecules (9 Hrs)

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

4.2 Macromolecules: Molecular mass- different averages, relation between different averages, calculation of different averages, methods of molecular mass determination- osmotic pressure, viscosity, sedimentation and light scattering methods.

Module 5: Photochemistry (18 Hrs)

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

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

5.3 Quenching of fluorescence and its kinetics, Stern-Volmer equation, concentration quenching, fluorescence and structure, delayed fluorescence, E-type and P-type, effect of temperature on emissions, photochemistry of environment, green house effect, two photon absorption spectroscopy, lasers in photochemical kinetics.

References

[1] J. Rajaram, J.C. Kuriakose, Kinetics and Mechanisms of Chemical Transformations, Macmillan India, 2000.

[2] K.J. Laidler, Chemical kinetics, 3rd Edn., Harper & Row, 1987.

[3] C. Kalidas, Chemical Kinetic Methods: Principles of Fast Reaction Techniques and Applications, New Age International, 2005.

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PG3ANL C12 –SPECTROSCOPIC METHODS IN CHEMISTRY

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

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

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

1.2 Influence of substituent, ring size and strain on spectral characteristics. Solvent effect, Stereochemical effect, non-conjugated interactions.

1.3 Problems based on the above topics.

1.4 Chirooptical properties- ORD, CD, octant rule, axial haloketone rule, Cotton effect.

Module 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.

Module 3: Nuclear Magnetic Resonance Spectroscopy (18 Hrs)

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

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

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

3.4 2D NMR and COSY, HOMOCOSY and HETEROCOSY

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

3.6 Problems on spectral interpretation with examples.

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

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

4.2 Problems on spectral interpretation with examples.

Module 5: Structure Elucidation Using Spectroscopic Techniques **(9 Hrs)**

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

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

References

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

[2] A.U. Rahman, M.I. Choudhary, Solving Problems with NMR Spectroscopy, Academic Press, 1996.

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

[12] Online spectral databases including RIO-DB.

[13] P.S. Kalsi. Spectroscopy of Organic Compounds, 5th Edn., New Age International, 2004.

SEMESTER 4

ELECTIVE COURSES

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

PG4ANL E01 ANALYTICAL PROCEDURES

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

Module 1: Errors in Chemical Analysis (18 Hrs)

Systematic and random errors. Distribution of experimental results. Statistical treatment- standard deviation, variance, confidence limits, application of statistics to data treatment and evaluation, student-t and f tests, detection of gross errors, rejection of a result-Q test, estimation of detection limits. Least square method, correlation coefficient and its determination. Hypothesis testing using statistical analysis.Using spread sheets for plotting calibration curves. Quality assurance and control charts.

Module 2: Conventional Analytical Procedures (18 Hrs)

2.1 Gravimetry: Inorganic precipitating agents: NH_3, H_2S, H_2SO_4, H_2PtCl_6, $H_2C_2O_4$, $(NH_4)_2MoO_4$ and NH_4SCN. Organic precipitating agents: oxine, cupron, cupferron, 1-nitroso-l-naphthol, BPHA, dithiocarbamates, sodium tetra phenyl boron, nioxime and nitron.

2.2 Acid base titrations in non-aqueous media. Different solvents and their selection for a titration. Indicators for non-aqueous titrations. Applications. Precipitation reactions-titration curves, determination of end points (coloured precipitates, colored soluble compounds), adsorption indicators, turbidity methods. Typical examples.

2.3 Redox titrations: Variation of potential during redox titrations, formal potential, requirements of redox titrations, detection of end point, typical titrants, $KMnO_4$, $K_2Cr_2O_7$, Ce (IV).

2.4 Complexometric titrations: masking and demasking agents, selective demasking, metal ion indicators, theory of visual use of metal indicators, typical examples of titrants - murexide, eriochrome black T.

Module 3: Sampling **(18 Hrs)**

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

3.2 Decomposition and dissolution, source of error, reagents for decomposition and dissolution, microwave decompositions, combustion methods, uses of fluxes. Elimination of interference from samples-separation by precipitation, electrolytic precipitation, extraction and ion exchange. Distribution ratio and completeness of multiple extractions.

Module 4: Applied Analysis **(18 Hrs)**

4.1 Analytical procedures involved in environmental monitoring. Water quality- Drinking water standards, BOD, COD, DO, nitrite, nitrate, iron, fluoride. Analysis of metal and radioactive pollutants in effluents.

4.2 Soil- moisture, salinity, colloids, cation and anion exchange capacity. Measurement of soil solution pH, Chemical and biochemical processes that influence soil solution pH.

4.3 Air pollution monitoring sampling, collection of air pollutants-SO_2, NO_2, NH_3, O_3 analysis of NO_2, SO_2, H_2S, O_3, CO, CO_2, NH_3, PM10 and PM 2.5. Air pollution monitoring instruments and monitoring programs

4.4 Analysis of metals, alloys and minerals. Analysis of brass and steel. Analysis of limestone. Corrosion analysis - weight loss and impedance methods.

4.5 Food and drug analysis: Food adulteration – common adulterants in food, coding of food colours. Pesticide analysis in food products. Analysis of alcoholic beverages. Analysis of drugs and pharmaceuticals: Quality control. Official methods. Classical and modern methods of drug analysis.

Module 5: Nano Materials **(9 Hrs)**

General introduction to nano materials and emergence of nano technology. Moore's law. Graphene (elementary ideas only), synthesis properties and applications of fullerenes and carbon nano tubes, synthesis of nano particles of gold, silver, rhodium, palladium and platinum techniques of synthesis electroplating and electrophoretic deposition conversion through chemical reactions and lithography. Thin films, chemical vapour deposition and atomic layer deposition techniques. Applications of nanoparticles.

Module 6: Chemical safety and toxicology (9 Hrs)

6.1 Hazards of handling ordinary, corrosive and poisonous chemicals.

6.2 Fire hazards. Handling carcinogens. Toxicology and residual analysis of Cd, Pb, Hg, As, Se and Pu (Atomic Absorption Spectroscopy). Toxicology of benzene, halogenated hydrocarbons, aromatic amino compounds, benzopyrene and related compounds. Treatment of hazardous waste and their disposal.

6.3 Radiochemical wastes-technique of safe disposal of radiochemical wastes.

6.4 Good Laboratory Practices.

References

[1] J.M. Mermet, M. Otto, R. Kellner, Analytical chemistry, Wiley-VCH, 2004.

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

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[15] T. Pradeep, Nano: the Essentials, Tata McGraw Hill, 2007.

[16] K.W. Kolasinski, Surface Science: Foundations of Catalysis and Nanoscience, 2nd Edn., Wiley, 2009.

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[18] W. Horwitz (Editor), Official Method of Analysis of AOAC International, 18th Edn., AOAC, 2010

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[20] B. K. Sharma. Environmental Chemistry, Goel Pub. Meerut.

[21] A. K. De Environmental Science Wily and Eastern Hd, N. Delhi.

PG4ANL E02 INSTRUMENTAL METHODS OF ANALYSIS

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

Module 1: Introduction to Instrumental Methods (18 Hrs)

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

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

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

Module 2: Molecular Spectral Measurements (18 Hrs)

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

2.2 Molecular fluorescence and fluorometers: photoluminescence and concentration electron transition in photoluminescence, factors affecting fluorescence, instrumentation details. Fluorometric standards and reagents. Applications in qualitative and quantitative analysis,

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

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

2.5 NMR spectrometry-magnets, shim coils, sample spinning; sample probes (^{1}H, ^{13}C, ^{31}P). Principle of MRI.

Module 3: Atomic Spectral Measurements (18 Hrs)

Atomic emission and atomic absorption phenomena: comparison of relative merits and drawbacks. Instrumentation details of AAS. Atomisation methods -flame, electrothermal and plasma techniques, glow discharge and laser ablation, sources: HCL, EDL-TGL, wavelength choice detectors, use in qualitative and quantitative analysis, interferences in measurements-chemical, spectral, and instrumental background correction techniques. Atomic emission spectroscopy flame, arc, spark, plasma emissions (ICP and DCP), details of wave selection detection systems, applications.

Module 4: Atomic X-ray spectrometry (9 Hrs)

Emission of X-ray, absorption process, fluorescence, instrumentation: X-ray tube, radio isotope filters and monochromators, X-ray detectors and transducers, photon counting, gas filled transducers, Geiger tube, counters, signal processors. Application in quantitative and qualitative analysis. Diffraction methods.

Module 5: Mass Spectrometry (9 Hrs)

Ion sources - EI, CI, FI, MALDI, Electrospray and FAB, Instrumental components-mass analyzers, magnetic sector, double focussing, quadrupole, TOF, Ion trap, FT instruments. Applications in identification of pure compounds, molecular formula, compound identification from comparison spectra, analysis of mixturesby hyphenated methods, quantitative applications. Application of MS with GC, HPLC.

Module 6: Surface Study Techniques - Instrumentation and Applications (9 Hrs)

6.1 Spectroscopic methods: ISS, SIMS, ESCA, AES, AAS.

6.2 Microscopic methods: SEM, TEM, STM, AFM.

Module7: Research Methodology of Chemistry (9 Hrs)

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

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

7.3 Chemical literature: primary, secondary and tertiary sources of literature. Classical and comprehensive reference. Literature databases: Science Direct, Sci Finder. Chemical Abstract.

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

7.5 Important scientific and chemistry journals. Impact factor.

References

[1] D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College Pub., 2007.

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PG4ANL E03 MODERN ANALYTICAL TECHNIQUES AND GREEN CHEMISTRY

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

Module 1: Electro Analytical Methods (27 Hrs)

1.1 Potentiometry: techniques based on potential measurements, direct potentiometric systems, different types of indicator electrodes, limitations of glass electrode, applications in pH measurements, modern modifications, other types of ion selective electrodes, solid, liquid, gas sensing and specific types of electrodes, biomembrane, biological and biocatalytic electrodes as biosensors, importance of selectivity coefficients. CHEMFETS- importance of specially designed amplifier systems for ion selective electrode systems. Potentiometric titrations- types and applications.

1.2 Polarography and voltametric techniques: micro electrode and their specialities, potential and current variations at the micro electrode systems, DME. Polarographic maxima, quantitative polarography, differential pulse square wave polarographic techniques. Applications of polarography. Cyclic voltametry: fundamental studies, study of redox systems using cyclic voltametry.

1.3 Amperometry: biamperometry, amperometric titrations. Coulometry-primary and secondary coulometry, advantages of coulometric titrations, applications. Principle of chronopotentiometry. Anodic stripping voltammetry- different types of electrodes and improvements of lower detection limits. Voltammetric sensors. Organic polarography.

Module 2: Capillary Electrophoresis and Capillary Electro Chromatography (9 Hrs)

2.1 Capillary electrophoresis-migration rates and plate heights, instrumentation, sample introduction, detection methods, applications. Capillary gel electrophoresis. Capillary isotachophoresis. Isoelectric focusing.

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

Module 3: Thermal and Radiochemical Methods (9 Hrs)

3.1 Thermogravimetry (TG), Differential Thermal Analysis (DTA) and Differential Scanning Calorimetry (DSC) and their instrumentation. Thermometric Titrations. Thermo Mechanical Analysis (TMA) and Dialatometric Analysis (DA)

3.2 Measurement of alpha, beta, and gamma radiations, neutron activation analysis and its applications. Principle and applications of isotope dilution methods, radiometric titrations.

Module 4: Chromatography (27 Hrs)

4.1 Classification, migration rates of solutes, important relationships Gas chromatography, GSC and GLC Instrumentation-preparation of column and column materials, temperature, effects, different types of detectors, capillary columns-bonded and cross linked phases, chiral stationary phases, selectivity factors, applications.

4.2 Liquid Chromatography: column efficiency, band broadening and the factors affecting it, particle size. HPLC- its instrumentation pumps, sample injection, columns, solvent selection and detectors. Partition chromatography- bonded phase.

4.3 Ion exchange chromatography-ion exchange equilibria, packings, detectors, applications.

4.4 Size Exclusion Chromatography- columns and limits of permeation and exclusion, applications.

4.5 Planar Chromatography-methodology, materials for stationary phases, applications. Paper chromatography.

4.6 Supercritical fluid chromatography: properties of supercritical fluids, operating variables in instrumentation, stationary and mobile phases, comparison with the techniques, applications, supercritical fluid extraction, advantages, applications.

Module 5: Process Instrumentation (9 Hrs)

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

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

6.1 Principles of green chemistry, atom economy, principles of green organic synthesis, green alternatives of organic synthesis-coenzyme catalysed reactions, green alternatives of molecular rearrangements, electrophilic aromatic substitution reactions, oxidation-reduction reactions, clay catalysed synthesis, condensation reactions. Green photochemical reactions.

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

6.3 General principles of microwave assisted organic synthesis.

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[1] J.M. Mermet, M. Otto, R. Kellner, Analytical Chemistry, Wiley-VCH, 2004.

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PG4ANL E04 - POLYMER CHEMISTRY

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

Module 1: Introduction to Polymer Science (9 Hrs)

1.1 History of macromolecular science: monomers, functionality, degree of polymerization, classification of polymers based on origin, structure, backbone, branching, action of heat, ultimate form and use, tacticity and crystalline behaviour.

1.2 Primary bonds-molecular forces in polymers: dipole forces, induction forces, dispersion forces and H bond, dependence of physical properties on intermolecular forces. Polymer molecular weight-different averages, polydispersity index, molecular weight distribution curve, polymer fractionation. Methods for molecular weight determination: end group analysis, colligative property measurements, ultracentrifugation, vapour phase osmometry, viscometry, GPC, light scattering method. Monomers and structure of common polymers like PE, PP, PVC, PVAc, PVA, PMMA, PEMA, poly lactic acid, PET, PBT, PS, PTFE, PEI, nylon 6, nylon 66, nylon 612, Kevlar, PEEK, PES, PC, ABS, PAN, PEO, PPO, PEG, SAN, PCL, PLA, PHB, DGEBA, MF, UF, AF, PF, PU, NR, SBR, NBR, PB, butyl rubber, polychloroprene and thiokol rubber.

Module 2: Fundamentals of Polymerization (18 Hrs)

2.1 Addition polymerization, free radical addition polymerization, mechanism and kinetics of vinyl polymerization, kinetics of free radical addition polymerization, effect of temperature, pressure, enthalpies, entropies, free energies and activation energies on polymerization.

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

2.3 Mechanism of coordination polymerization, Ziegler-Natta polymerization, ring opening polymerization, mechanism of polymerization of cyclic amides.

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

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

2.6 Controlled polymerization methods, nitroxide mediated polymerization, Ring Opening polymerization (ROP), Atom Transfer Radical Polymerization (ATRP), Reversible Addition Fragmentation Termination (RAFT).

Module 3: Properties of Polymers (18 Hrs)

3.1 Structure property relationship in polymers, transitions in polymers, first order and second order transitions in polymers, relationship between Tg and Tm, molecular motion and transitions, Boyer-Beamem rule, factors affecting glass transition temperature.

3.2 Rheological properties of polymers, Newtonian fluids, non-Newtonian fluids, pseudoplastic, thixotropy, St. Venant body, dialatant, complex rheological fluids, rheopectic fluids, time dependent fluids, time independent fluids, power law, Weissenberg effect, laminar flow, turbulent flow, die swell, shark skin, viscous flow.

3.3 Viscoelastic properties of polymers, viscoelasticity, Hooke's law, Newton's equation, viscoelastic models-time temperature equivalence, WLF equation, Boltzmann superposition principle, linear stress - strain relations for other types of deformation-creep, stress relaxation. Temperature dependence of viscosity. Transport in polymers - diffusion, liquid and gas transport, Fick's law, theories of diffusion.

Module 4: Stereochemistry and Conformation of Polymers (9 Hrs)

4.1 Stereoregular polymers, constitutional isomerism, positional isomerism and branching, optical isomerism, geometric isomerism, substitutional isomerism, configuration of polymer chains, infrared, Raman and NMR characterization, polymer conformation, chain end to end distance, random walks and random flights, self-avoiding walks.

Module 5: Morphology and Order in Crystalline Polymers (9 Hrs)

5.1 Polymer morphology, common polymer morphologies, structural requirements for crystallinity, degree of crystallinity, crystallisability- mechanism of crystallization, polymer single crystals, lamellar structure of polymers, fringed micelle concept, folded chain model, adjacent re-entry model, switchboard model.

5.2 Structure of polymers crystallised from melt, spherulitic morphology, mechanism of spherulite formation, theories of crystallisation kinetics, Avrami equation, Hoffman's nucleation theory, the entropic barrier theory, strain induced morphology, cold drawing, morphology changes during orientation, application of XRD, SEM and DSC in determining the crystallinity of polymers.

Module 6: Advances in Polymers (9 Hrs)

6.1 Specialty polymers, conducting polymers, high temperature polymers, flame resistant polymers, biopolymers and biomaterials, polymers in medicine, polymers for dental applications.

6.2 Carbon fibres. Synthesis, characterization and applications of carbon nanofibres.

Module 7: Dendrimers and Dendritic Polymers (18 Hrs)

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

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

7.3 Characterisation of dendrimers: GPC, osmosis, TG, DSC, magnetic resonance spectroscopy (proton and carbon-13 NMR), mass spectral studies(MALDI and TOF).

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

References

[1] V.R. Gowariker, N.V. Viswanathan, J. Sreedhar, Polymer Science, New Age International, 2003.

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[3] L. H. Sperling, Introduction to Physical Polymer Science, 4thEdn, John Wiley & Sons, 2006.

[4] J.M.G. Cowie, V. Arrighi, Polymers: Chemistry and Physics of Modern Materials, 3rd Edn., CRC Press, 2008.

[5] D.I. Bower, An Introduction to Polymer Physics, Cambridge University Press, 2002.

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[12] H.R. Allock, F. W. Lampe, Contemporary Polymer Chemistry, Pearson/Prentice Hall, 2003.

PG4ANL E05 APPLIED ANALYSIS AND AQUATIC RESOURCES

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

Module 1: Environmental Analysis (18 Hrs)

1.1 Water Analysis: sampling and preservation of water. Determination of pH, EC,TDS, DO, CO_2, alkalinity (carbonate, bicarbonate, hydroxide and total), salinity, chloride, fluoride, sulphate, H_2S, calcium, magnesium, sodium, potassium, iron (total ferrous and ferric), ammonia, nitrite, nitrate, phosphorous (total inorganic and organic), BOD, COD, phenols, surfactants, pesticides, E-Coli and total bacteria. Quality of water, standards of raw and treated water, objectives of waste water treatment. A brief idea of sedimentation, coagulation and flocculation, filtration, disinfection of water. Activated sludge process, trickling filters, sludge treatment and disposal. Softening of water, corrosion and its control. Removal of toxic compounds, refractory organics, and dissolved inorganic substances. Reverse osmosis.

1.2 Air Analysis: atmospheric pollution, classification of air pollutants, sources of air pollution and methods of control, sampling of aerosols, sampling of gaseous pollutants, analysis of SO_x, NO_x, CO-CO_2, hydrocarbons, particulates, effects of air pollutants on animals, ozone layer, chlorofluorocarbons, acid rain, greenhouse effect.

1.3 Soil/Sediment analysis: a brief idea of chemistry of soil. Trace element analysis in soil - B, Cd, Cu, Fe, Mn, Mo, Zn, Pb. Pesticides and pollution, classification and degradation of pesticides, methods of pesticides analysis. Sampling of soil, aquatic sediments, pH, electrical conductivity, redox potential, alkalinity, inorganic and organic contents.

1.4 Waste Management: waste management approaches - waste reduction, recycling, disposal. Management of hazardous wastes, household waste, municipal and industrial wastes-collection, transportation and disposal options.

Module 2: Biochemical and Clinical Analysis (9 Hrs)

2.1 Cell fractionation techniques-cell lysine: differential and density gradient centrifugation, salting in, salting out, dialysis, ultracentrifugation, electrophoretic techniques-polyacrilamide gel electrophoresis, SDS-PAGE, agrose gel electrophoresis.

2.2 Liver function tests, gastric function tests, kidney function tests and glucose tolerance tests. Screening of metabolic diseases.

Module 3: Forensic Analysis (18 Hrs)

3.1 Forensics-basic principles and significance, history and development. Crime-definition, crime scene, protection and recording of crime scene, physical clues, processing of crime scene.

3.2 Finger prints: classification, conventional methods of development of finger prints-fluorescent and chemical methods. Application of laser and other radiations to development of latent finger print. Foot prints, tyre marks, bite marks and lip prints.

3.3 Questioned Document Examination (QDE): forged documents and currency notes. UV counterfeit note detector.

3.4 Forensic Ballistics-fire arms, classification and characteristics, analysis of gunshot residues, mechanism of GSR, instrumental methods of GSR analysis.

3.5 Explosives: introduction, types, preliminary screening at crime scene, presumptive test (colour and spot test), micro chemical methods of analysis.

3.6 Fire Extinguishers and its chemistry, analysis of Arson exhibits by instrumental methods, management of flammable and combustible materials.

3.7 Counterfeit coins- AAS analysis, purity of Gold-analysis by XRF / EDXRF.

3.8 Forensic Toxicology: classification of poisons, estimation of poisons and drugs with chromatographic, neutron activation analysis and spectrophotometric methods.

Module 4: Food Chemistry and Food Analysis (36 Hrs)

4.1 Food chemistry: definition and importance. Water in food, water activity and shelf life of food. Carbohydrates-chemical reactions, functional properties of sugars and polysaccharides in foods. Lipids: classification and use of lipids in foods, physical and chemical properties, effects of processing on functional properties and nutritive value. Protein and amino acids-physical and chemical properties, distribution, amount and functions of proteins in foods, functional properties, effect of processing-loss of vitamins and minerals due to processing. Pigments in food, food flavours, browning reaction in foods. Enzymes in foods and food industry, bio-deterioration of foods, food contaminants, additives and toxicants.

4.2 Principles of food processing: scope and importance of food processing. Principles and methods of food preservation-freezing, heating, dehydration, canning, addition of additives, fermentation, irradiation, extrusion cooking, hydrostatic pressure cooking, dielectric heating, microwave processing, aseptic processing, hurdle technology, membrane technology. Storage of food-modified atmosphere packaging, refrigeration, freezing and drying of food, minimal processing, radiation processing.

4.3 Food microbiology: history of microbiology of food, microbial growth pattern, physical and chemical factors influencing destruction of micro-organisms. Types of micro-organisms normally associated with food-mold, yeast and bacteria. Micro-organisms in natural food products and their control. Contaminants of food-stuffs, vegetables, cereals, pulses, oil seeds, milk and meat during handling and processing. Biochemical changes caused by micro-organisms, deterioration of various types of food product. Food poisoning and microbial toxins, microbial food fermentation, standards for different foods. Food borne intoxicants and mycotoxins.

4.4 Advanced techniques of food analysis: role of analysis and various methods of sampling and analysis of results. Principles and application of flame photometry, atomic absorption, X-ray analysis, electrophoresis, mass spectroscopy, NMR, chromatography, refractometry, rheology, measurements, enzymatic methods, DSC, SEM, rapid methods of microbial analysis, immunoassays, ESR.

Module 5: Aquatic Resources (9 Hrs)

5.1 Aquatic resources: renewable and non-renewable resources-estimation, primary productivity, regional variations. Desalination: principles and applications of desalination-distillation, solar evaporation, freezing, electrodialysis, reverse osmosis, ion-exchange and hydrate formation methods. Relative advantages and limitations of the methods. Scale formation and its prevention in distillation process.

5.2 Non-renewable resources: inorganic chemicals from the sea-extraction and recovery of halides, magnesium, potassium, gold.

References

[1] B.B. Nanda, R.K. Tewari, Forensic Science in India: A Vision for the Twenty- first Century, Select Pub., 2001.

[2] A.S. Osborn, Questioned Documents, 2nd Edn., Rawman & Littlefield Pub., 1974.

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[19] H. Wright, A Hand book of Soil Analysis, Logos Press, 1994.

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SEMESTER 3 & 4

PG4ANL P04– INORGANIC CHEMISTRY PRACTICAL – 2

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

PART I

Estimation of simple binary mixtures (like Cu-Ni, Cu-Zn, Fe-Cr, Fe-Cu, Fe-Ni, Pb-Ca) of metallic ions in solution by volumetric and gravimetric methods.

PART II

Analysis of one of the alloys of brass, bronze and solder. Analysis of one of the ores from hematite, chromite, dolomite, monazite, illmenite.

References

[1] A.I. Vogel, A Text Book of Quantitative Inorganic Analysis, Longman, 1966.

[2] I.M. Koltoff, E.B. Sandell, Text Book of Quantitative Inorganic Analysis, 3rd Edn., Mc Millian, 1968.

[3] G. Pass, H. Sutcliffe, Practical Inorganic Chemistry, Chapman & Hall, 1974.

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PG4ANL P05 ORGANIC CHEMISTRY PRACTICAL - 2

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

PART I

A. Volumetric estimation of 1) Aniline 2) Phenol 3) glucose 4) Iodine value and saponification value of coconut oil

B. Colorimetric estimation of 1) Aniline 2) Glucose 3) Cholesterol 4) ascorbic acid 5) Streptomycin 6) Aspirin.

C. Estimation of the number of acetyl, methoxy, phenolic, amino, nitro, carboxyl, ester, ether and carbonyl groups in organic compounds.

PART II

Preparation of compounds by two stages.

1. Acetanilide- p-nitroacetanilide-- p-nitroaniline
2. Methyl benzoate-- -m-nitromethylbenzoate-- m-nitrobenzoic acid
3. Acetanilide- p-bromoacetanilide-- p-bromoaniline
4. Phenol-salicylaldehyde-coumarin
5. Benzophenone –benzophenone oxime- benzanilide
6. Aniline -2,4,6-tribromoaniline-1,3,5-tribromoaniline

PART III

1. Microwave assisted Organic Synthesis.
2. Preparation Involving by the Green alternatives of Chemical Methods.

PART IV

Prediction of FTIR, UV-Visible, ^{1}H and ^{13}C NMR spectra of the substrates and products at each stage of the products synthesized by the above methods.

PART V – Viva-Voce

References

[1] A.I. Vogel, A Textbook of Practical Organic Chemistry, Longman, 1974.

[2] A.I. Vogel, Elementary Practical Organic Chemistry, Longman, 1958.

[3] F.G. Mann and B.C Saunders, Practical Organic Chemistry, 4th Edn., Pearson Education India, 2009.

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PG4ANL P06 INSTRUMENTAL ANALYSIS PRACTICAL

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

Section A

I. Nephelometry

1. Determination of sulphate.
2. Determination of halides.

II. UV – Visible Spectrophotometry

1. Determination of absorption curve and concentration of a substance (Potassium nitrate)
2. Simultaneous determination of Ti^{3+} and V^{5+} spectrophotometrically by H_2O_2 method.
3. Spectrophotometric determination of the pK value of an indicator (the acid dissociation constant of methyl red)
4. Determination of phenols in water

III. Polarimetry

1. Kinetics of the inversion of sucrose in presence of HCl.
2. Determination of the concentration of a sugar solution
3. Determination of the concentration of HCl.
4. Determination of the relative strength of acids.

IV. Refractometry

1. Identification of pure organic liquids and oils.
2. Determination of molar refractions of pure liquids.
3. Determination of concentration of solutions (KCl-water, glycerol-water)
4. Determination of molar refraction of solids.
5. Study of complex formation between potassium iodide and mercuric iodide system.

Section B

V. Polarography and related experiments.

1. Determination of half wave potential.
2. Determination of Cd by (a) standard series (b) Standard addition (c) pilot ion method.
3. Determination of organic compounds.

VI. Conductivity measurements

1. Verification of Onsager equation.
2. Determination of the degree of ionization of weak electrolytes.
3. Determination of pKa values of organic acids.
4. Determination of solubility of sparingly soluble salts.
5. Titration of a mixture of acids against a strong base.
6. Titration of a dibasic acid against a strong base.

VII. Potentiometry

1. Determination of single electrode potentials (Cu and Zn)
2. Application of Henderson equation.
3. Potentiometric titrations, pH metric titrations.
4. Determination of the concentration of a mixture of Cl^- and I^- ions.

VIII. Electrogravimetric estimation of Cu, Ni, and Pb

IX. Flame Photometry

Determination of Na^+, Li^+, K^+ and Ca^{2+}.

The examination will be for 6 hours with one experiment each from section A and section B and will have equal weight.

References

[1] J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.
[2] B. Viswanathan, Practical Physical Chemistry, Viva Pub., 2005.
[3] G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th Edn., McGraw Hill, 2009.
[4] A. Findlay, Practical Physical chemistry, Longman.
[5] F. Daniels et al Experimental Physical chemistry, McGraw Hill.
[6] Shoemaker, Garlands, Experiments in Physical chemistry, McGraw Hill.

M.Sc. PHARMACEUTICAL CHEMISTRY

M.Sc. PHARMACEUTICAL CHEMISTRY

	Code	Course	Hours/ week	Total Hours	Credit	Marks		
						Internal	External	Total
Semester 1	PG1PHA C01	Inorganic Chemistry-I (Coordination & Nuclear Chemistry)	4	72	4	20	80	100
	PG1PHA C02	Organic Chemistry-I (Structure, Reactivity & Stereochemistry)	4	72	4	20	80	100
	PG1PHA C03	Theoretical Chemistry-I (Quantum Chemistry and Group Theory)	4	72	4	20	80	100
	PG1PHA C04	Physical chemistry- I (Kinetic Theory, Thermodynamics and Statistical Thermodynamics)	3	54	3	20	80	100
	PG2PHA P01	Inorganic Chemistry Practical–1	3	54	Evaluation at the end of second semester			
	PG2PHA P02	Organic Chemistry Practical-1	3	54				
	PG2PHA P03	Physical Chemistry Practical -1	4	72				
		Total	**25**	**450**	**15**			
Semester 2	PG2PHA C05	Inorganic Chemistry-II (Bioinorganic & Organometallic Chemistry)	4	72	4	20	80	100
	PG2PHA C06	Organic Chemistry- II (Reaction Mechanism)	4	72	4	20	80	100
	PG2PHA C07	Theoretical Chemistry – II (Chemical Bonding and Computational Chemistry)	4	72	4	20	80	100
	PG2PHA C08	Physical chemistry- II (Molecular Spectroscopy)	3	54	3	20	80	100
	PG2PHA P01	Inorganic Chemistry Practical–1	3	54	3	20	80	100
	PG2PHA P02	Organic Chemistry Practical-1	3	54	3	20	80	100
	PG2PHA P03	Physical Chemistry Practical -1	4	72	4	20	80	100
		Total	**25**	**450**	**25**			

Semester 3	PG3PHA C09	Organic Chemistry- II (Synthetic and Bioorganic Chemistry)	4	72	4	20	80	100
	PG3PHA C10	Physical chemistry – III (Advanced Topics in Physical Chemistry)	4	72	4	20	80	100
	PG3PHA C11	Medicinal Chemistry- I (Drug Design and Pharmacolocgy)	4	72	4	20	80	100
	PG3PHA C12	Spectroscopic Methods in Chemistry	3	54	3	20	80	100
	PG4PHA P04	Pharmaceutical Analysis and Pharmacognosy Practical	3	54	Evaluation at the end of fourth semester			
	PG4PHA P05	Drug Synthesis and Dispensing Practical	3	54				
	PG4PHA P06	Biochemistry and Bacteriology Practical	4	72				
		Total	**25**	**450**	**15**			
Semester 4	PG4PHA E01	Elective 1Bacteriology and Biochemistry	5	90	4	20	80	100
	PG4PHA E02	Elective 2 Pharmacognosy and Pharmaceutical Operations	5	90	4	20	80	100
	PG4PHA E03	Elective 3 Medicinal Chemistry- II	5	90	4	20	80	100
	PG4PHA E04	Elective 4 Polymer Chemistry	5	90	4	20	80	100
	PG4PHA E05	Elective 5 Analytical Chemistry	5	90	4	20	80	100
	PG4PHA P04	Pharmaceutical Analysis and Pharmacognosy Practical	3	54	3	20	80	100
	PG4PHA P05	Drug Synthesis and Dispensing Practical	3	54	3	20	80	100
	PG4PHA P06	Biochemistry and Bacteriology Practical	4	72	3	20	80	100
	PG4PHA D01	Project			2	20	80	100
	PG4PHA V01	Viva			2	20	80	100
		Total	**25**	**450**	**25**			
Grand Total					**80**			

SEMESTER 1

PG1PHA C01 INORGANIC CHEMISTRY – I

(COORDINATION & NUCLEAR CHEMISTRY)

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

Module 1: Coordination Chemistry- Structural Aspects and Bonding (18 Hrs)

1.1 Classification of complexes based on coordination numbers and possible geometries. σ and π bonding ligands such as CO, NO, CN^-, R_3P and Ar_3P.

1.2 Splitting of *d* orbitals in octahedral, tetrahedral, square planar, square pyramidal and trigonal 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 with and without π-bonding, experimental evidences for π-bonding

Module 2: Kinetics and Mechanism of Reactions in Metal Complexes (18 Hrs)

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

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

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

Module 3: Organometallic Compounds- Synthesis, Structure and Bonding (18 Hrs)

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

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

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

Module 4: Electron deficient compounds **(9 Hrs)**

Electron deficient compounds – synthesis, reactions, structure and bonding. Boron hydrides, styx numbers, Boron cluster compounds.

Wade's rule, Hydroborate anions, Organoboranes and hydroboration, Polyhedral anions, Carboranes, Metalloboranes, Borazines and Borides.

Module 5: Nuclear Chemistry **(9 Hrs)**

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

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

5.3 Analytical applications of radioisotopes- radiometric titrations, kinetics of exchange reactions, measurement of physical constants including diffusion constants, neutron activation analysis, prompt gamma neutron activation analysis and neutron absorptiometry.

5.4 Applications of radio isotopes in industry, medicine, autoradiography, radiopharmacology, radiation safety precaution, nuclear waste disposal.

5.5 Radiation chemistry of water and aqueous solutions- Fricke solution, Ceric ammonium solution. Measurement of radiation doses. Relevance of radiation chemistry in biology, organic compounds and radiation polymerization.

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[9] S.N. Goshal, Nuclear Physics, S. Chand and Company, 2006.

PG1PHA C02 ORGANIC CHEMISTRY - I

(STRUCTURE, REACTIVITY & STEREOCHEMISTRY)

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

Module 1: MO Theory and Aromaticity (9 Hrs)

1.1 Review of basic concepts in organic chemistry: bonding, hybridization, MO picture (allyl system, 1,3-butadiene and benzene), inductive effect, electromeric effect, resonance effect, hyperconjugation, steric effect. Bonding weaker than covalent bonds.

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

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

Module 2: Investigation of Organic Reaction Mechanisms (9 Hrs)

Energy profiles, Methods of determining reaction mechanisms, Kinetic and thermodynamic control of reactions. The Hammond postulate. Principle of microscopic reversibility. Marcus theory. The Hammett equation and its applications. Taft equation. Linear free energy relationships. Solvent polarity and parameters. Y, Z and E parameters and their applications. Primary and secondary kinetic isotope effects. Salt effects and special salt effects in SN reactions. Solvent effect. Bulk and specific solvent effects. Introduction to carbon acids - pKa of weak acids, kinetic and thermodynamic acidity. Phase transfer catalysis and its applications. Steric effects. HSAB principle and its applications in organic reactions.

Module 3: Review of Organic Reaction Mechanisms (18 Hrs)

3.1 Review of organic reaction mechanisms with special reference to nucleophilic and electrophilic substitution at aliphatic carbon (S_N1, S_N2, S_Ni, S_E1, S_E2, addition-elimination and elimination-addition sequences), elimination (E1 and E2). Elimination vs substitution.

3.2 A comprehensive study on the effect of substrate, reagent, leaving group, solvent and neighbouring group on nucleophilic substitution (S_N2 and S_N1) and elimination (E1 and E2) reactions.

3.3 Addition reactions (regioselectivity- Markovnikov's addition- carbocation mechanism, anti-Markovnikov's addition- radical mechanism).

3.4 Mechanism of electrophilic and nucleophilic aromatic substitution reactions with examples. Arenium ion intermediates. S_N1, S_NAr, $S_{RN}1$ and Benzyne mechanisms.

3.5 Catalysis by acids, bases and nucleophiles with examples from acetal, cyanhydrin and ester formation and hydrolysis reactions- $A_{AC}2$, $A_{AC}1$, $A_{AL}1$, $B_{AC}2$ and $B_{AL}1$ mechanisms.

Module 4: Stereochemistry of Organic Compounds (18 Hrs)

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

4.2 Stereoisomerism: Definition based on symmetry and energy criteria, configurational and conformational stereoisomers.

4.3 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 C_n, molecules with more than one center of chirality, definition of diastereoisomers, constitutionally symmetrical and unsymmetrical chiral molecules, erythro and threo nomenclature.

4.4 Axial, planar and helical chirality with examples, stereochemistry and absolute configuration of allenes, biphenyls, binaphthyls, ansa and cyclophanic compounds, spiranes, exocyclic alkylidene cycloalkanes.

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

4.6 Geometrical isomerism: Nomenclature, E-Z notation, methods of determination of geometrical isomers. Interconversion of geometrical isomers.

Module 5: Conformational Analysis (18 Hrs)

5.1 Conformational descriptors- factors affecting conformational stability of molecules. Conformational analysis of acyclic and cyclic systems: substituted ethanes, cyclohexane and its derivatives, decalins, adamantane, congressane, sucrose and lactose. Fused and bridged bicyclic systems.

5.2 Conformation and reactivity of elimination (dehalogenation, dehydrohalogenation, semipinacolic deamination and pyrolytic elimination- Saytzeff and Hofmann eliminations), substitution and oxidation of 2° alcohols. Chemical consequence of conformational equilibrium - Curtin Hammett principle. Chiral drugs.

References

[1] R. Bruckner, Advanced Organic Chemistry: Reaction Mechanisms, Academic Press, 2002.

[2] I. Fleming, Frontier Orbitals and Organic Chemical Reactions, Wiley, 1976.

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PG1PHA C03 THEORETICAL CHEMISTRY – I

(QUANTUM CHEMISTRY AND GROUP THEORY)

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

Module 1: Formulation of Quantum Chemistry (18 Hrs)

1.1 Mathematical Concepts (5 Hrs)

Co-ordinate systems: Cartesian, Cylindrical polar and Spherical polar coordinates and their relationships. Complex numbers: definition, Complex conjugate, absolute value of a complex number, complex functions. Operator algebra: linear and nonlinear operators, Hermitian operators, del and del-squared operators. Eigen function and eigen values of an operator, Eigen value equation, Eigen functions of Commuting operators. Well behaved functions, Normalized and Orthogonal functions.

1.2 Evolution of Quantum Mechanics (5 Hrs)

Failure of classical mechanics: The black body radiation, Compton effect, photoelectric effect, atomic spectra. Need of quantum mechanics. Concept of matter wave, de Broglie relation and its experimental proof, Uncertainty principle and its consequences. Wave function and Born interpretation, Schrödinger's wave mechanics, Deduction of Schrodinger equation from classical wave equation.

1.3 Postulates of Quantum Mechanics (4 Hrs)

Detailed discussion of postulates: State function postulate. Operator postulate. Eigen value postulate. Expectation value postulate. Postulate of time dependent Schrodinger equation of motion, Conservative system and time-independent Schrodinger equation.

1.4 Quantum Mechanics of Translational Motion (4 Hrs)

Particle in one-dimension with infinite potential walls, particle in a three dimensional box- separation of variables- rectangular box and cubic box, degeneracy. Introduction to tunnelling with experimental evidence.

Module 2: Applications of Quantum Chemistry (18 Hrs)

2.1 Quantum Mechanics of Hydrogen-like Atoms (5 Hrs)

Potential energy of hydrogen-like systems. The wave equation in spherical polar

coordinates: separation of variables- R, Θ and Φ equations and their solutions, wave functions and energies of hydrogen-like atoms. Orbitals- radial functions, radial distribution functions, angular functions and their plots.

2.2 Quantum Mechanics of Vibrational Motion (5 Hrs)

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. Rodrigue's formula, Three dimensional harmonic oscillator.

2.3 Quantum Mechanics of Rotational Motion (5 Hrs)

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 Φ equation and its solution, wave functions in the real form. Non-planar rigid rotor (or particle on a sphere)- separation of variables, the Φ and the Θ equations and their solutions, Legendre and associated Legendre equations, Legendre and associated Legendre polynomials. Spherical harmonics (imaginary and real forms)- polar diagrams of spherical harmonics.

2.4 Orbital and Spin angular momentum (3 Hrs)

Quantisation of angular momentum, quantum mechanical operators corresponding to angular momenta, (L_x, L_y, L_z and L^2). Commutation relations between these operators. Spherical harmonics as eigen functions of angular momentum operators L_z and L^2. Space quantization. The postulate of spin by Uhlenbeck and Goudsmith, discovery of spin- Stern Gerlach experiment. Spin orbitals- construction of spin orbitals from orbital and spin functions.

Module 3: Molecular Symmetry and Mathematical group (18 Hrs)

3.1 Symmetry elements and symmetry operations. Conditions for a set of elements to form a group, sub groups, abelian and cyclic groups, Point groups. Multiplication of operations. Group multiplication table of C_{2v}, C_{2h} and C_{3v} groups (H_2O, Trans N_2F_2 and NH_3 as examples). Similarity transformation and classes in a group.

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

3.3 Reducible and Irreducible representations (IR). Reduction formula, reduction of reducible representation to IRs.

Module 4: Applications of Group Theory (18 Hrs)

4.1 The Great Orthogonality theorem. Rules derived from GOT (proof not required). Setting up of character table of C_{2v}, C_{3v}, C_{2h}, C_{4v} and C_3 groups. Direct product representations.

4.2 Applications in quantum mechanics, transition moment integral, vanishing of integrals. Jahn – Teller effect, Woodward – Hoffmann rules.

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

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

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PG1PHA C04 - PHYSICAL CHEMISTRY - I

(KINETIC THEORY, THERMODYNAMICS AND STATISTICAL THERMODYNAMICS)

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

Module 1: Kinetic theory (9 Hrs)

Kinetic theory of gases, 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, transport properties of gases. Viscosity, thermal conductivity and diffusion. Determination of viscosity of gases. Influence of temperature and pressure on transport properties.

Module 2: Classical Thermodynamics (18 Hrs)

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

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

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

2.4 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.

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

2.6 Chemical affinity and thermodynamic functions, effect of temperature and pressure on chemical equilibrium- van't Hoff reaction isochore and isotherm.

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

2.8 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, and three pairs of partially miscible liquids.

Module 3: Irreversible Thermodynamics and Bioenergetics (9 Hrs)

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

Module 4: Statistical Thermodynamics (18 Hrs)

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

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

References

[1] P.W. Atkins, Physical Chemistry, ELBS, 1994.

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SEMESTER 2

PG2PHA C05 INORGANIC CHEMISTRY- II

(BIOINORGANIC & ORGANOMETALLIC CHEMISTRY)

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

Module 1: Acids, Bases and Non-aqueous solvents (9 Hrs)

1.1 Acid base concept in non-aqueous media-HSAB concept, solvent effect, linear free energy relationship- mechanism and method of determination.

1.2 Reaction in non-aqueous solvents. Ammonia- solution of metals in liquid ammonia. Protonic solvents: anhydrous sulphuric acid, hydrogen halide. Aprotic solvents: non-polar solvents, non-ionizable polar solvents. Polar solvents undergoing autoionization. Liquid halogen, Inter halogen compounds, oxy halides, dinitrogen tetroxide, sulphur dioxide.

Module 2: Bioinorganic Compounds (18 Hrs)

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

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

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

Module 3: Spectral and Magnetic Properties of Metal Complexes (18 Hrs)

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

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

3.3 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.

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

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

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

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

Module 5: Stereochemistry of Coordination Compounds (9 Hrs)

5.1 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.

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

Module 6: Reactions of Organometallic Compounds (9 Hrs)

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

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

6.3 Rearrangement reactions, redistribution reactions, fluxional isomerism.

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

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

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PG2PHA C06 ORGANIC CHEMISTRY - II

(REACTION MECHANISM)

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

Module 1: Chemistry of Carbocations (9 Hrs)

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

1.2 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, Demjanov rearrangement. Oxymercuration, halolactonisation.

Module 2: Chemistry of Carbanions (18 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, Kinetic and thermodynamic enolates- Lithium and boron enolates in Michael and aldol reactions, alkylation and acylation of enolates. Chemistry of enamines, Stork-Enamine reaction.

2.2 Nucleophilic additions to carbonyls groups. Reactions involving carbanions-mechanisms of Claisen, Dieckmann, Knoevenagel, Stobbe, Darzen and acyloin condensations, Shapiro reaction and Julia elimination. Favorskii rearrangement.

2.3 Reactions of carbonyl compounds: oxidation, reduction (Clemmensen and Wolff-Kishner), addition reactions (addition of cyanide, ammonia, alcohol), Aldol condensation, Cannizzaro reaction, addition of Grignard reagent.

2.4 Structure and reactions of α, β- unsaturated carbonyl compounds involving electrophilic and nucleophilic addition- Michael addition, Mannich reaction, Robinson annulation.

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

Module 3: Carbenes, Carbenoids, Nitrenes and Arynes (9 Hrs)

3.1 Generation, structure and reactions of carbenes. Rearrangement reactions of carbenes: Wolff rearrangement, generation and reactions of ylids by carbenoid decomposition.

3.2 Structure, generation and reactions of nitrenes. Hoffmann, Curtius, Lossen, Schmidt and Beckmann rearrangement reactions.

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

Module 4: Radical Reactions (9 Hrs)

4.1 Generation and detection 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. Autoxidation.

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

Module 5: Concerted reactions (18 Hrs)

5.1 Symmetry properties of molecular orbitals of ethylene and conjugated systems with three or more atoms, Woodward – Hoffmann rule, Conservation of orbital symmetry and stereo chemical courses.

5.2 Pericyclic reactions like Electrocyclic (butadiene-cyclobutene and hexatriene-cyclohexadiene interconversions), Cycloadditions (2+2) & (4+2), Sigmatropic (1,3), (1,5) and (3,3), Cheletropic including Cheletropic eliminations and Ene reaction with stereo chemical aspects.

5.3 Diels- Alder reactions with stereochemical aspects.

5.4 Analysis of Pericyclic Reactions. (i) FMO method (ii) Orbital- correlation method and (iii) PMO method.

5.2 Highlighting pericyclic reactions in organic synthesis such as Claisen, Cope, Mislow-Evans, Wittig and Sommelet-Hauser rearrangements. dipolar cycloaddition (introductory). Unimolecular pyrolytic elimination reactions, decomposition of

cyclic azo compounds, β-eliminations involving cyclic transition states such as N-oxides, acetates and xanthates.

Module 6: Organic Photochemistry (9 Hrs)

6.1 Photochemical processes. Energy transfer. Jablonski diagram, sensitization and quenching. Singlet and triplet states and their reactivity.

6.2 Photoreactions of carbonyl compounds, enes, dienes and arenes. Norrish reactions of acyclic ketones. Patterno-Buchi, Barton, Photo-Fries and Di-л methane rearrangements. Photoreactions of Vitamin D. Photosynthesis and photochemistry of vision. Singlet oxygen generation and their reactions.

References

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PG2PHA C07 THEORETICAL CHEMISTRY - II

(CHEMICAL BONDING AND COMPUTATIONAL CHEMISTRY)

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

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

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

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

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

Module 2: Chemical Bonding (18 Hrs)

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

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

2.3 Hybridization, quantum mechanical treatment of sp, sp^2 and sp^3 hybridisation. Semiempirical MO treatment of planar conjugated molecules, Hückel Molecular

Orbital (HMO) theory of ethene, allyl systems, butadiene and benzene. Calculation of charge distributions, bond order and free valency.

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

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

Module 4: Computational Chemistry (18 Hrs)

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

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

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

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

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

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

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

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

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

Module 5: Computational Chemistry Calculations (9 Hrs)

5.1 Molecular geometry input-cartesian coordinates and internal coordinates, Z-matrix. Z-matrix of: single atom, diatomic molecule, non-linear triatomic molecule, linear triatomic molecule, polyatomic molecules like ammonia, methane, ethane and butane. General format of GAMESS/Firefly input file. GAMESS/Firefly key word for: basis set selection, method selection, charge, multiplicity, single point energy calculation, geometry optimization, constrained optimization and frequency calculation.

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

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

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Softwares

Molecular Mechanics:

01. **Arguslab** available from www.arguslab.com/
02. **Tinker** available from www.dasher.wustl.edu/ffe/

Ab initio, semiempirical and dft:

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

Graphical User Interface (GUI):

01. **Gabedit** available from http://gabedit.sourceforge.net/
02. **wxMacMolPlt** available from http://www.scl.ameslab.gov/MacMolPlt/
03. **Avogadro** from http://avogadro.openmolecules.net/wiki/Get_Avogadro

PG2PHA C08 PHYSICAL CHEMISTRY - II

(MOLECULAR SPECTROSCOPY)

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

Module 1: Microwave and Infrared Spectroscopy (18 Hrs)

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

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

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

Module 2: Electronic, Mossbauer and Raman spectroscopy (18 Hrs)

2.1 Electronic spectroscopy: Term symbols of diatomic molecules, electronic spectra of diatomic molecules, selection rules, vibrational coarse structure and rotational fine structure of electronic spectrum, Franck-Condon principle, predissociation, calculation of heat of dissociation, Birge and Sponer method, electronic spectra of polyatomic molecules, spectra of transitions localized in a bond or group, free electron model.

Different types of lasers- solid state lasers, continuous wave lasers, gas lasers and chemical laser, frequency doubling, applications of lasers, introduction to UV and X-ray photoelectron spectroscopy.

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

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

Module 3: Resonance Spectroscopy (18 Hrs)

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

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

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

3.4 An elementary study of NQR spectroscopy.

References

[1] C.N. Banwell, E.M. McCash, Fundamentals of Molecular Spectroscopy, 4^{th} Edn., Tata McGraw Hill, 1994.

[2] G. Aruldhas, Molecular Structure and Spectroscopy, Prentice Hall of India, 2001.

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SEMESTERS 1 AND 2

PG2PHA P01 INORGANIC CHEMISTRY PRACTICAL – 1

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

PART I

Separation and identification of four metal ions of which two are rare/ less familiar such as Tl, W, V, Se, Te, Ti, Ce, Th, Zr, U, Mo and Li and common cations - 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+}, Co^{2+}, Ni^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}, Mg^{2+}, Li^{+}, Na^{+}, K^{+}, NH_4^{+} (interfering acid radicals are not present). Confirmation by spot test (Minimum **8** mixtures are to be recorded).

PART II

1. Argentometric estimation of chlorides
2. Cerimetry – Fe(II) and nitrate
3. Potassium iodate – iodide estimation of Sn(II)

PART III

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

PART IV

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

1. Tris (thiourea) copper (I) complex
2. Potassium tris (oxalate) aluminate (III)
3. Tetrammine copper (II) sulphate
4. Mercury tetra thiocyanato cobaltate (III)

References

[1] A.I. Vogel, A Text Book of Qualitative Inorganic Analysis Including Elementary Instrumental Analysis, 3rd Edn., ELBS.

[2] G. Svelha, Text Book of Vogel's Macro and Semi-micro Inorganic Analysis, revised, Orient Longman.

[3] V.V. Ramanujam, Inorganic Semi micro Qualitative Analysis, The National Publishing Co., Chennai.

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

PG2PHA P02 ORGANIC CHEMISTRY PRACTICAL - 1

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

PART I

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

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

PART II

A. Separation of organic binary mixtures:- 1. Quantitative separation of a mixture oftwo components by solvent extraction 2. Purification of the separated samples by distilling and crystallization. 3. Determination of physical constants of separated and purified samples (No need of bifunctional compounds).

B. Separation of organic mixtures by TLC and calculation of R_f values.

C. Separation/purification of organic mixtures by column chromatography.

PART III

Drawing the structures of organic molecules and reaction schemes and mechanisms by ChemDraw, SymyxDraw and Chemsketch.

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

PART IV- Viva voce

References

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PG2PHA P03 PHYSICAL CHEMISTRY PRACTICAL - 1

Credit: 4 **Contact Lab Hours: 72+72 =144**

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

Part A

I. Adsorption

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

II. Phase diagrams

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

III. Distribution law

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

IV. Surface tension

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

Part B
Computational Chemistry Experiments

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

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

References

[1] J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.
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SEMESTER 3

PG3PHA C09 ORGANIC CHEMISTRY- III

(SYNTHETIC AND BIOORGANIC CHEMISTRY)

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

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

1.1 Survey of organic reagents and reactions in organic chemistry with special reference to oxidation. Metal based and non-metal based oxidations of (a) alcohols to carbonyls (chromium, manganese, aluminium, and silver based reagents) (b) phenols (Fremy's salt, silver carbonate) (c) alkenes to epoxides (peroxides/peracids based), Sharpless asymmetric epoxidation (d) alkenes to diols (Manganese, Osmium based), Sharpless asymmetric dihydroxylation, Prevost reaction (e) alkenes to carbonyls with bond cleavage (manganese, osmium, ruthenium and lead based, ozonolysis) (f) alkenes to alcohols/carbonyls without bond cleavage (hydroboration-oxidation, Wacker oxidation) (g) ketones to ester/lactones (Baeyer-Villiger).

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

Module 2: Modern Synthetic Methods (9 Hrs)

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

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

Module 3: Stereoselective Transformations (9 Hrs)

3.1 Asymmetric induction-chiral auxiliaries and chiral pool.

3.2 Enantioselective catalytic hydrogenation developed by Noyori and Knowels.

3.3 Asymmetric aldol condensation pioneered by Evans.

3.4 Asymmetric Diels-Alder reactions.

3.5 Asymmetric epoxidation using Jacobsen's catalyst.

Module 4: Construction of Ring Systems (9 Hrs)

4.1 Different approaches towards the synthesis of three, four, five and six-membered rings- Pauson-Khand reaction, Bergman cyclization, Nazarov cyclization, cation-olefin cyclization and radical-olefin cyclization. Ring closing metathesis.

4.2 Structure and formation of heterocyclic rings: 5-and 6-membered ring heterocyclic compounds with one or more than one hetero atom like N, S or O- pyrrole, furan, thiophene, imidazole, pyrazole, thiazole, oxazole, pyridine, purines and pyrimidines, quinoline and isoquinoline.

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

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

5.2 Molecular receptors: Cyclodextrins, Crown ethers, Cryptands, Tweezers, Carcerands, Cyclophanes, Calixaranes, carbon nanocapsules.

5.3 Importance of molecular recognition in biological systems.

5.4 Applications of supramolecular complexes in medicine and perfumery industries.

Module 6: Chemistry of Natural Products and Biomolecules (18 Hrs)

6.1 Terpenoids: Classification of terpenoids. Synthesis of camphor. Biogenesis of isoprenoids.

6.2 Steroids: classification and nomenclature of steroids. Reactions, structure elucidation, stereochemistry and biosynthesis of cholesterol. Structure and semi synthesis of steroid hormones- testosterone, estrogen and progesterone. Biosynthesis of steroids.

6.3 Alkaloids: Classification of alkaloids, general methods of structure elucidation of alkaloids. Structure elucidation and synthesis of papaverine, quinine and morphine. Stereoselective synthesis of reserpine. Biosynthesis of alkaloids- papaverine, morphine.

6.4 Vitamins: classification and structure of vitamins A, B_1, B_2, B_6, and C. Synthesis of vitamins A, C, B_1 and B_2.

6.5 Natural colouring species: anthocyanins and carotenoids, structure and synthesis of cyanin, flavone, quercetine and β-carotene.

6.6 Basic principles of the biosynthesis of terpenes, carbohydrates, proteins and nucleic acids. Biomimetic synthesis of progesterone and spatriene.

References

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[20] P. S. Kalsi, Sangeeta Jagtap, Pharmaceutical, Medicinal and Natural Product Chemistry, Alpha Science, 2013

PG3PHA C10 PHYSICAL CHEMISTRY- III

(ADVANCED TOPICS IN PHYSICAL CHEMISTRY)

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

Module 1: Electrochemistry and Electromotive Force (9 Hrs)

1.1 Theories of ions in solution, Drude and Nernst's electrostriction model and Born's model, Debye-Huckel theory, Derivation of Debye-Huckel-Onsager equation, validity of DHO equation for aqueous and non aqueous solutions, Debye-Falkenhagen effect, conductance with high potential gradients, activity and activity coefficients in electrolytic solutions, ionic strength, Debye-Huckel limiting law and its various forms, qualitative and quantitative tests of Debye- Huckel limiting equation, deviations from the DHLL.

Module 2: Chemical Kinetics (18 Hrs)

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

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

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

Module 3: Surface Chemistry and Colloids (18 Hrs)

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

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

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

Module 4: Quantum Statistics (9 Hrs)

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

4.2 Heat capacity of solids- Dulong and Petit’s law, the vibrational properties of solids, Einsteins theory- Derivation, and its limitations, Debye theory – derivation and its limitations.

Module 5: Photochemistry (18 Hrs)

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

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

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

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PG3PHA C11 MEDICINAL CHEMISTRY – I

(DRUG DESIGN & PHARMACOLOGY)

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

Module 1: Drug Discovery, Design and Development (27 Hrs)

1.1 Development of new drugs: Lead discovery, Random screening, rational approaches, sources of lead compounds, methods of lead discovery, lead modification, identification of pharmacophore, functional group modification, structure-activity relationships, drug-like molecules, structure modification to increase potency-homologation, chain branching, ring chain transformation, bioisosterism, combinatorial chemistry-general aspects, solid – phase mix and split synthesis, parallel chemical synthesis and encoding techniques. Structure modification to increase oral bioavailability- electronic effects, lipophilicity effects.

1.2 Quantitative structure activity relationships: Steric effects, Hansch analysis, de novo method, Topliss method. Computer–Based Methods of QSAR, Basic concepts of CADD, molecular modeling, molecular docking. Introduction to 2D & 3D QSAR. (18 Hrs)

1.3 Retrosynthetic analysis: Introduction to Retrosynthetic analysis and disconnection approach-synthetic strategy and synthons- Retrosynthetic analysis of benzocaine, saccharin, salbutamol and benzodiazepines. (5 Hrs)

1.4 Receptors: Classification of receptors, Drug- receptor interactions, Theories of Drug-receptor interactions, stereochemical aspects, drug–receptor chirality, geometrical isomers, conformational isomers, ring topology. (4 Hrs)

Module 2: Basic principles of Drug Design and Pharmacology (9 Hrs)

2.1 General principles of pharmacology: Drug nomenclature, orphan drugs, Concept of prodrugs and soft drugs. Routes of drug administration, biological response to drugs.

2.2 Pharmacokinetic principles: Passage of drugs across membranes, absorption, distribution, metabolism-Phase I and Phase II reactions, and excretion of drugs.

2.3 Pharmacodynamic principles: Principles of drug action, mechanism of drug action, dose- response relationships, drug selectivity, unusual and adverse responses of drugs, structurally specific and nonspecific drugs.

2.4 Drug interactions: Synergism, antagonism, drug addiction, drug abuse, drug dependence, drug tolerance, drug hypersensitivity, Immunoglobulins.

Module 3: Inorganic pharmaceutical chemistry (9 Hrs)

3.1 Preparation and uses of the following compounds used in pharmacy: Aluminium hydroxide gel, calcium lactate, calcium gluconate, ferrous fumarate, ferric ammonium citrate, ferrous sulphate, calamine, zinc oxide, zinc stearate, magnesium stearate, talc, yellow mercuric oxide, trivalent and pentavalent antimonials, selenium sulfide, lithium salts, gold, platinum and bismuth compounds,metal complexes used in medicine.

3.2 Metal toxicity - cadmium, lead, copper and mercury.

Study of the chemistry, SAR and uses of the following classes of compounds. Synthesis needed only for the mentioned compounds.

Module 4: Drugs acting on CNS (18 Hrs)

4.1 General anaesthetics: Inhalation anaesthetics - ether, enflurane, halothane, nitrous oxide, cyclopropane. Intravenous anaesthetics–thiopentone sodium, ketamine.

4.2 Hypnotics, sedatives and anxiolytic agents: Barbiturates, benzodiazepines, and miscellaneous- chlordiazepoxide, meprobamate. Anxiolytic agents-benzodiazepines, buspirone, meprobamate.

4.3 Anticonvulsants: Convulsions, types of epilepsy, barbiturates, hydantoins, oxazolidinediones, succinimides, benzodiazepines.

4.4 Analeptics: Xanthines, amphetamines, nikethamide and ethamivan.

4.5 Tranquilisers: Rauwolfia alkaloids, meprobamate, oxazepam, benzodiazepines, chlordiazepoxide, phenothiazene derivatives.

4.6 Antidepressants: MAO inhibitors- Isocarboxazide, tranylcypromine and phenelzine. Tricyclic compounds -imipramine, amitriptyline. Miscellaneous compounds- fluoxetine and trazodone.

4.7 Antipsychotics: Phenothiazine derivatives, thiothixene derivatives, butyrophenone derivatives- haloperidol, rauwolfia alkaloids.

4.8 Hallucinogens: Triptamine derivatives- DMT, psilocybin, phenylalkylamines- mescaline, Lysergic acid derivatives-LSD, Cannabinol compounds.

4.9 Synthesis of the following drugs: Enflurane, Phenobarbital, Chlordiazepoxide, Buspirone, Nikethamide.

Module 5: Analgesics and Antipyretics (9 Hrs)

5.1 Narcotic analgesics: morphine and its analogues, phenyl (ethyl) piperidines, diphenyl heptanones and benzazocin derivatives.

5.2 Antipyretics and NSAIDs: Basic idea of COX I & COX II inhibitors, salicylates- aspirin; p-aminophenol derivatives- paracetamol; pyrazolidinedione derivatives– phenylbutazone, oxyphenbutazone; anthranilic acid derivatives- mefanamic acid, flufenamic acid; indoleacetic acid derivatives- indomethacin; arylacetic/propionic acid derivatives- ibuprofen, and diclofenac; oxicams – piroxicam; selective COX II inhibitors-celecoxib.

5.3 Anti- gout drugs: allopurinol, colchicine.

5.4 Centrally acting muscle relaxants: glyceryl ethers- mephenesin; alkanediol derivatives- meprobamate; benzodiazepines-librium, diazepam; miscellaneous compounds-baclofen.

5.5 Synthesis of the following drugs: Meperidine, phenylbutazone, flufenamic acid, diclofenac, piroxicam and celicoxib.

References

[1] Richard B. Silverman, The Organic chemistry of drug Design and Drug Action, 2nd Edn. Academic Press, Elsevier, 2004.

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PG3PHA C12 SPECTROSCOPIC METHODS IN CHEMISTRY

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

Module1: 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.

1.3 Problems based on the above topics.

1.4 Chirooptical properties-ORD, CD, octant rule, axial halo ketone rule, Cotton effect.

Module 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.

Module 3: Nuclear Magnetic Resonance Spectroscopy (18 Hrs)

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

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

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

3.4 2D NMR and COSY, HOMOCOSY and HETEROCOSY

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

3.6 Problems on spectral interpretation with examples.

Module 4: Mass Spectrometry (9 Hrs)

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

4.2 Problems on spectral interpretation with examples.

Module 5: Structural Elucidation Using Spectroscopic Techniques (9 Hrs)

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

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

References

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SEMESTER 4

ELECTIVE COURSES

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

PG4PHA E01 BACTERIOLOGY AND BIOCHEMISTRY

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

Module 1: Introduction to Microbiology (9 Hrs)

1.1 A general study of viruses, fungi and protozoa. Morphology, classification and scientific nomenclature of bacteria. Growth requirements of bacteria. Classification of nutrient media. Applications of nutrient media in the practice of bacteriology. Staining of bacteria, theories of staining. Viral infections, methods of viral multiplication, causing of diseases, bacteriophages. General principles of microbial control- sterilization, disinfection, prions.

1.2 Cells- classification and cell division

Module 2: Immunity (9 Hrs)

Types of immunity. Antigens and antibodies: theories of antigen-antibody reactions, AIDS, applications of antigen-antibody reactions. Interferons. Vaccines and sera - general study of the preparation of different types of vaccines, sera and toxoids. Monoclonal antibodies.

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

3.1 Amino acids and Proteins: Essential amino acids. Primary structure of proteins and amino acid analysis. Ramachandran plot and secondary structure of proteins. Tertiary structure and structural motifs- protein folding and domain structure of proteins. Quaternary structure of proteins. Purification and characterization of proteins. Functions of proteins. Chemical synthesis of proteins- protecting groups, solution and solid phase peptide synthesis.

3.2 Nucleic acids: DNA and RNA. Double helical structure of DNA. Replication of DNA. Classification of RNA. Genetic code. Nucleic acids as carriers of genetic information. Protein biosynthesis. Transcription, translation, DNA finger printing technique. Elementary principles of Recombinant DNA technology, gene therapy, cloning and bioinformatics. Human genome project, DNA profiling and Polymerase chain reaction.

Module 4: Enzymes and Hormones (18 Hrs)

4.1 Enzymes: 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.

4.2 Hormones: Functions and modes of actions of hormones. Pituitary, thyroid, parathyroid, pancreatic, adrenal and adrenocortical hormones. Male and female sex hormones. Antihormones.

Module 5: Metabolism (18 Hrs)

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

5.2 Lipid metabolism: β-oxidation of fatty acids. Ketogenesis and ketosis. Biosynthesis of fatty acids. Essential fatty acids. Prostaglandins- nomenclature, structure and biosynthesis.

5.3 Metabolism of amino acids and proteins: Oxidative deamination and transamination reactions. Urea formation- ornithine cycle. Inborn errors of metabolism.

Module 6: Biological Oxidation and Electron Transport Chain (9 Hrs)

6.1 Biological Oxidation: High energy compounds, ATP and ADP. Substrate level and oxidative phosphorylation. Electron transport chain, Cytochromes.

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

Module 7: Blood Composition and Acid Base Balance (9 Hrs)

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

7.2 Regulation of acid base balance. Acidosis and alkalosis. Renal function. Formation and composition of urine. Diabetes insipidus.

References

[1] D.M. Vasudevan, S. Sreekumari, V. Kannan, Textbook of Biochemistry for Medical Students, 6th Edn., JAYPEE Medical Publishers(P) Ltd., 2010.

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PG4PHA E02 PHARMACOGNOSY & PHARMACEUTICAL OPERATIONS

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

Module 1: Pharmacognosy-1 **(18 Hrs)**

Pharmacognosy of the official drugs frequently used in pharmacy: Names, sources, chemical constituents, macroscopial characters and uses of senna, belladona, digitalis, stramonium, vasaka, cinnamon, cinchona, ergot, ipecacuanha, rauwolfia, liquorice, ginger, cloves, pyrethrum, santonica, nutmeg, nuxvomica, cardamom, umbelliferous fruits like Cumin, Fennel, Caraway, Opium, Aloes, Asafoetida, Vinca rosea, Brahmi (two varieties).

Module 2: Pharmacognosy-II **(9 Hrs)**

2.1 Fixed oils and essential oils used in pharmacy-their sources. Extraction, constituents, composition and analysis of fixed oils. Elementary study of adulteration of fixed oils.

2.2 Fixed Oils: Castor oil, Olive oil, Shark liver oil, cod liver oil.

2.3 Essential Oils: Eucalyptus oil, Turpentine oil. Uses of essential oils in medicine – Aromatherapy.

2.4 A brief study of the substances used as pharmaceutical necessities – Starches, gum acacia, gum tragacanth, agar- agar, gelatin, talc, kaolin, bentonite and white petroleum jelly, wools fat, lanolin, bees wax, yellow bees wax.

Module 3: Dispensing **(9 Hrs)**

3.1 Principles of dispensing medicaments. Incompatibilities and overcoming of incompatibilities. Preparation of pills, tablets, capsules, injectables, emulsions, suppositories, coating of tablets.

3.2 Newer Drug Delivery systems: Site specific drug delivery systems – to brain, CNS, GIT, kidney and urinary tract and in cancer chemotherapy, controlled release phenomena, slow release phenomena, implanted mechanical pumps.

Module 4: Forensic Pharmacy (18 Hrs)

4.1 Pharmaceutical Legislation in India. Legal aspects of trade in drugs. The drug Act and Drug rules. The Pharmacy Act. The dangerous drug Act and Rules. The Drugs and Cosmetic Act and rules

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

4.3 Intellectual Property Rights (IPR), Patents, Trademarks, Copy rights, Patent Acts relevant sections (basic ideas only).

Module 5: Pharmaceutical Operations (18 Hrs)

5.1 Principles involved, Apparatus and machinery used in general pharmaceutical operations of IP/BP - evaporation, extraction, crystallization, distillation.

5.2 Chromatographic techniques: theory of chromatography, Applications of adsorption, partition, paper, thin layer and column chromatographic methods. LC, HPLC, IEC, GC and GPC. Column matrices. Detectors. Affinity and chiral columns.

5.3 Electrophoresis - general ideas. Ultracentrifugation.

5.4 Solvent extraction, liquid – liquid extraction, uses of oxine, dithiazone, dithiocarbamates, high molecular weight amines and crown ethers in extraction.

Module 6: Nanotechnology and Green Chemistry (9 Hrs)

6.1 Applications of nanomaterials in medicine: immunogold labelling, applications in medical diagnosis, nano based drug delivery, biomimetic nanotechnology, DNA nanotechnology and structural biomimicry.

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

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

6.4 Green chemistry in pharmaceutical industry: Ibuprofen manufacture, bio-catalysis.

Module 7: Polymers and Diagnostic agents (9 Hrs)

7.1 Conducting polymers, Polymers for NLO applications, Polymers for medical applications, Dendrimers- Methods of synthesis, dendrimers as nanocapsules, Applications of dendrimers. Biopolymers and their medical applications.

7.2 Radiopaques – organoiodo compounds. Compounds used in function tests, dyes, radio isotopes, RIA, ELISA, blotting techniques, finger printing studies of DNA.

7.3 Dyes used in pharmacy: fluorescein, mercurochrome, acridine dyes.

7.4 Colouring agents: official colours, colour code.

7.5 Liver and gastric function tests and kidney function tests.

References

[1] T.E. Wallis, Text Book of Pharmacognosy, 5th Edn., J & A Churchil, 1967.

[2] W.C. Evans, Trease and Evans' Pharmacognosy, 15th Edn., Bailliere Tindall, 2002.

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PG4PHA E03 MEDICINAL CHEMISTRY- II

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

Module1: Drugs acting on ANS **(18 Hrs)**

1.1 Adrenergic stimulants: α- and β- adrenoreceptor agonists, Phenyl ethanolamine derivatives-adrenaline, isoprenaline, salbutamol, ephedrine, and phenylephrine. Imidazoline derivatives- naphazoline, xylometazoline and oxymetazoline.

1.2 Adrenergic blockers: α- and β- adrenoreceptor antagonists- ergot alkaloids, phenoxybenzamine, tolazoline, propranolol, atenolol, labetolol. Neuron blockers– bretylium and xylocholine.

1.3 Cholinergic stimulants: Nicotinic and muscarinic receptors, acetylcholine and analogues, pilocarpine, bethanechol and carbachol.

1.4 Cholinergic blockers: Tertiary and quaternary antimuscarinics. Antispasmodic drugs-dicyclomine, glycopyrrolate. Antiulcer drugs- pirenzepine. Cycloplegic drugs-tropicamide, homatropine.

1.5 Anticholinesterases: Competitive inhibitors- physostigmine and neostigmine. Non-competitive inhibitors- organophosphorus compounds, Nerve gases, Cholinesterase regenerators- 2 PAM.

1.6 Antiparkinson's agents: Dopamine agonists, dopamine releasing agents and synthetic anticholinergics. Drugs for Alzheimer's disease: Cholinergic agonists and acetylcholinesterase inhibitors.

1.7 Curare form drugs: Curare alkaloids, erythrina alkaloids and gallamine.

1.8 Synthesis of the following drugs: Salbutamol, carbachol, tolazoline, propranolol.

Module 2: Drugs acting on CVS **(18Hrs)**

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

2.2 Antiarrhythmic drugs: Classification, quinidine, disopyramide, lidocaine, phenytoin and procainamide, β-blockers-propranolol. Calcium channel blockers-verapamil and neuron blockers- bretylium.

2.3 Antihypertensive drugs: Classification, Peripheral antiadrenergics- prazosin and terazosin. Centrally acting drugs- reserpine, clonidine and methyl dopa. β-blockers- propranolol, atenolol and labetalol. Direct vasodilators- hydralazine and minoxidil. Ganglion blocking agents- mecamylamine and trimethophan. Calcium channel blockers- nifedipine and amlodipine. ACE inhibitors- captopril. Angiotensin receptor blockers- losartan. Diuretics- thiazide diuretics.

2.4 Antianginal drugs: Vasodilators- nitrites and nitrates, β-blockers- propranolol, atenolol, nadolol. Calcium channel blockers- verapamil and nifedipine. Miscellaneous- dipyridamole and aspirin.

2.5 Anticoagulants: Heparin, coumarin derivatives and indanedione derivatives.

2.6 Hypolipidaemic agents: Atherosclerosis (elementary idea only), Statins-lovastatin, fluvastatin, atorvastatin. Fibrates- clofibrate. Miscellaneous- bile acid sequestrants and cholestyramine resin and Gugulipid.

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

Module 3: Chemotherapy (18 Hrs)

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

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

3.3 Antimicobacterial agents: A brief study of infection, its development and social significance. Antitubercular agents: first line drugs- isoniazid, rifampicin, pyrazinamide, ethambutol, and streptomycin. Second line drugs- ethionamide, para aminosalicylic acid, kanamycin and fluoroquinolones. Types of leprosy, Antileprotic drugs- dapsone, phenazine derivatives- clofazimine.

3.4 Antifungal agents: Systemic and topical antifungal agents- Antibiotics- amphotericin B, griseofulvin and nystatin. Azole derivatives- ketoconozole, fluconozole and clotrimazole. Pyrimidine derivatives- 5- Flucytosine.

3.5 Antiviral drugs: A brief study of infection, its development and social significance. Principles of antiviral drugs. Nucleoside and non-nucleoside analogues. Anti-herpes virus drugs- Idoxuridine, vidarabine and acyclovir. Anti-retro virus drugs- zidovudine and abacavir. Anti-influenza virus drugs- amantadine, oseltamivir (tamiflu). Nonselective antiviral drugs- interferons and ribavirin.

3.6 Antiprotozoal agents: A brief study of infection, its development and social significance. Amoebicides: Ipecacuanha alkaloids- emetine, dehydroemetine, metranidazole and tinidazole. Antimalarials: Life cycle of parasite. 4-aminoquinolines, 8-amino quinolines, acridine and artemesinine derivatives. Anthelmintics: piperazines and benzimidazoles. Taeniasis- albendazole.

3.7 Synthesis of the following drugs: Ampicillin, cephalexin, chloramphenicol, sulphamethoxazole, dapsone, metronidazole.

Module 4: Antineoplastic Drugs (9 Hrs)

4.1 Neoplasm: cause, therapeutic approaches. Classification of drugs, Alkylating agents-nitrogen mustards, nitrosourea, aziridines and aryl sulphonates. Antimetabolites- folic acid antagonists, purine and pyrimidine antagonists. Antibiotics- anthracyclines, actinomycin D and bleomycin. Plant products- vinca alkaloids, taxol derivatives. Hormones and their antagonists- tamoxifen. Miscellaneous- procarbazine, cisplatin.

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

Module 5: Antihistaminic drugs and Gastrointestinal drugs (9Hrs)

5.1 Antihistaminic drugs: Histamine and its biological role, H_1 receptor antagonists- aminoalkyl ethers- diphenhydramine and doxylamine. Ethylenediamine derivatives-pyrilamine, phenothiazines- promethazine, trimeprazine, piperazine derivatives- cyclizine, miscellaneous compounds- cetrizine and cyproheptadine.

5.2 Drugs for peptic ulcer: Antacids- systemic and non- systemic antacids, H_2 receptor antagonists- cimetidine, ranitidine and famotidine. Proton pump inhibitors- omeprazole and pantoprazole. Anti-H.pylori drugs, Gastroesophageal reflux disease (GERD).

5.3 Purgatives: Irritant, osmotic, bulk and lubricant purgatives, digestants, carminatives and antidiarrhoeals.

5.3 Synthesis of the following drugs: Diphenhydramine, pyrilamine, promethazine, omeprazole.

Module 6: Miscellaneous class of compounds (18 Hrs)

6.1 Diuretics: Common diuretics and their mechanism of action. Mercurial and non-mercurial diuretics- carbonic anhydrase inhibitors- acetazolamide and methazolamide. Thiazide derivatives- hydrochlorothiazide, Sulphonamides, osmotic diuretics- mannitol, isosorbide, glycerol. Loop diuretics- furosemide and ethacrynic acid, potassium sparing diuretics- amiloride, spironolactone. Antidiuretics- antidiuretic hormone.

6.2 Oral hypogycemic agents: Type 1 and Type 2 diabetes, insulin, suphonylureas- tolbutamide, acetohexamide and glibenclamide, glipizide. biguanides-metformin, thiazolidinediones-rosiglitazone.

6.3 Local anaesthetics: Clinical application of local anaesthesia, coca and cocaine, hexylcaine, para amino benzoic acid derivatives- benzocaine, procaine, tetracaine, anilides, lidocaine.

6.4 Expectorants and Antitussives: Centrally acting antitussives- opium alkaloids and synthetic substitutes- codeine, noscapine, pholcodine, ethyl morphine, dextromethorphan. Expectorants- terpin hydrate, guaicol and bromhexine.

6.5 Synthesis of the following drugs: Acetazolamide, furosemide, ethacrynic acid, benzocaine, dextromethorphan.

References

[1] G.L. Patrick, Medicinal Chemistry, BIOS, 2001.

[2] T. Nogrady, D.F. Weaver, Medicinal Chemistry, Oxford University Press, 2005.

[3] W.O. Foye, T.L. Lemke, D.A. Williams, Principles of Medicinal Chemistry, 4th Edn., Williams & Wilkins, 1995.

[4] J.P. Remington, Remington's Pharmaceutical Sciences, Vol.13, 19th Edn., Mack,1990.

[5] D. Sriram, P.Yogeswari, Medicinal Chemistry, Pearson Education India, 2010.

[6] K.D. Tripathi, Essentials of medical Pharmacology, 6th Edn., Jaypee, 2008.

[7] L.S. Goodman, A. Gillman, The Pharmacological Basis of Therapeutics, 10th Edn., McGraw Hill, 2001.

[8] S.S. Kadam, Principles of Medicinal Chemistry, Vol. I& II, Pragati Books, 2008.

[9] A. Kar, Medicinal Chemistry, New Age International, 2007.

[10] C.O. Wilson, J.M. Beale, J. Block, Textbook of Organic Medicinal and Pharmaceutical Chemistry, 12th Edn., Lippincott Williams & Wilkins, 2010.

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PG4PHA E04 - POLYMER CHEMISTRY

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

Module 1: Introduction to Polymer Science **(9 Hrs)**

1.1 History of macromolecular science: monomers, functionality, degree of polymerization, classification of polymers based on origin, structure, backbone, branching, action of heat, ultimate form and use, tacticity and crystalline behaviour.

1.2 Primary bonds-molecular forces in polymers: dipole forces, induction forces, dispersion forces and H bond, dependence of physical properties on intermolecular forces. Polymer molecular weight-different averages, polydispersity index, molecular weight distribution curve, polymer fractionation. Methods for molecular weight determination: end group analysis, colligative property measurements, ultracentrifugation, vapour phase osmometry, viscometry, GPC, light scattering method. Monomers and structure of common polymers like PE, PP, PVC, PVAc, PVA, PMMA, PEMA, poly lactic acid, PET, PBT, PS, PTFE, PEI, nylon 6, nylon 66, nylon 612, Kevlar, PEEK, PES, PC, ABS, PAN, PEO, PPO, PEG, SAN, PCL, PLA, PHB, DGEBA, MF, UF, AF, PF, PU, NR, SBR, NBR, PB, butyl rubber, polychloroprene and thiokol rubber.

Module 2: Fundamentals of Polymerization **(18 Hrs)**

2.1 Addition polymerization, free radical addition polymerization, mechanism and kinetics of vinyl polymerization, kinetics of free radical addition polymerization, effect of temperature, pressure, enthalpies, entropies, free energies and activation energies on polymerization.

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

2.3 Mechanism of coordination polymerization, Ziegler-Natta polymerization, ring opening polymerization, mechanism of polymerization of cyclic amides.

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

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

2.6 Controlled polymerization methods, nitroxide mediated polymerization, Ring Opening polymerization (ROP), Atom Transfer Radical Polymerization (ATRP), Reversible Addition Fragmentation Termination (RAFT).

Module 3: Properties of Polymers (18 Hrs)

3.1 Structure property relationship in polymers, transitions in polymers, first order and second order transitions in polymers, relationship between Tg and Tm, molecular motion and transitions, Boyer-Beamem rule, factors affecting glass transition temperature.

3.2 Rheological properties of polymers, Newtonian fluids, non-Newtonian fluids, pseudoplastic, thixotropy, St. Venant body, dialatant, complex rheological fluids, rheopectic fluids, time dependent fluids, time independent fluids, power law, Weissenberg effect, laminar flow, turbulent flow, die swell, shark skin, viscous flow.

3.3 Viscoelastic properties of polymers, viscoelasticity, Hooke's law, Newton's equation, viscoelastic models-time temperature equivalence, WLF equation, Boltzmann superposition principle, linear stress - strain relations for other types of deformation-creep, stress relaxation. Temperature dependence of viscosity. Transport in polymers - diffusion, liquid and gas transport, Fick's law, theories of diffusion.

Module 4: Stereochemistry and Conformation of Polymers (9 Hrs)

Stereoregular polymers, constitutional isomerism, positional isomerism and branching, optical isomerism, geometric isomerism, substitutional isomerism, configuration of polymer chains, infrared, Raman and NMR characterization, polymer conformation, chain end to end distance, random walks and random flights, self-avoiding walks.

Module 5: Morphology and Order in Crystalline Polymers (9 Hrs)

5.1 Polymer morphology, common polymer morphologies, structural requirements for crystallinity, degree of crystallinity, crystallisability- mechanism of crystallization, polymer single crystals, lamellar structure of polymers, fringed micelle concept, folded chain model, adjacent re-entry model, switchboard model.

5.2 Structure of polymers crystallised from melt, spherulitic morphology, mechanism of spherulite formation, theories of crystallisation kinetics, Avrami equation, Hoffman's nucleation theory, the entropic barrier theory, strain induced morphology, cold drawing, morphology changes during orientation, application of XRD, SEM and DSC in determining the crystallinity of polymers.

Module 6: Advances in Polymers (9 Hrs)

6.1 Specialty polymers, conducting polymers, high temperature polymers, flame resistant polymers, biopolymers and biomaterials, polymers in medicine, polymers for dental applications

6.2 Carbon fibres. Synthesis, characterization and applications of carbon nanofibres.

Module 7: Dendrimers and Dendritic Polymers (18 Hrs)

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

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

7.3 Characterisation of dendrimers: GPC, osmosis, TG, DSC, magnetic resonance spectroscopy (proton and carbon-13 NMR), mass spectral studies (MALDI and TOF).

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

References

[1] V.R. Gowariker, N.V. Viswanathan, J. Sreedhar, Polymer Science, New Age International, 2003.

[2] F.W. Billmeyer Jr., Textbook of Polymer Science, 3rd Edn., Wiley-India, 2007.

[3] L. H. Sperling, Introduction to Physical Polymer Science, 4th Edn, John Wiley & Sons, 2006.

[4] J.M.G. Cowie, V. Arrighi, Polymers: Chemistry and Physics of Modern Materials, 3rd Edn., CRC Press, 2008.

[5] D.I. Bower, An Introduction to Polymer Physics, Cambridge University Press, 2002.

[6] M. Chanda, Introduction to Polymer Science and Chemistry: A Problem Solving approach, CRC/Taylor & Francis, 2006.

[7] P.J. Flory, Principles of Polymer Chemistry, Cornell University Press, 1983.

[8] J.R. Fried, Polymer Science and Technology, 2nd Edn., Prentice Hall, 2003.

[9] G. Odian, Principles of Polymerization, 4th Edn., John Wiley & Sons, 2007

[10] K.J. Saunders, Organic Polymer Chemistry, Chapmann & Hall, 1973.

[11] K. Matyjaszewski, T.P. Davis, Handbook of Radical Polymerization, John Wiley & Sons, 2003.

[12] H.R. Allock, F. W. Lampe, Contemporary Polymer Chemistry, Pearson/Prentice Hall, 2003.

PG4PHA E05 ANALYTICAL CHEMISTRY

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

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

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

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

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

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

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

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

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

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

Module 2: Sampling (18 hrs)

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

2.2 Decomposition and dissolution, source of error, reagents for decomposition and dissolution like HCl, H_2SO_4, HNO_3, $HClO_4$, HF, microwave decompositions, combustion methods, use of fluxes like Na_2CO_3, Na_2O_2, KNO_3, NaOH, $K_2S_2O_7$, B_2O_3 and lithium metaborate. Elimination of interference from samples-separation by precipitation, electrolytic precipitation, extraction and ion exchange.Distribution ratio and completeness of multiple extractions.Types of extraction procedures.

Module 3: Applied Analysis (9 hrs)

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

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

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

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

Module 4: Capillary Electrophoresis and Capillary Electro Chromatography (9 Hrs)

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

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

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

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

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

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

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

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

References

[1] J.M. Mermet, M. Otto, R. Kellner, Analytical Chemistry, Wiley-VCH, 2004.

[2] D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College Pub., 2007.

[3] R.D. Brownn, Introduction to Instrumental Analysis, McGraw-Hill, 1958.

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

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

[6] J.H. Kennedy, Analytical Chemistry: Principles, Saunders College Pub., 1990.

[7] J.G. Dick, Analytical Chemistry, R.E. Krieger Pub., 1978.

[8] E.D. Howe, Fundamentals of Water.

SEMESTERS 3 & 4

PG4PHA P04 PHARMACEUTICAL ANALYSIS & PHARMACOGNOSY PRACTICAL

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

PART I

Preparation, assay including limit tests prescribed in the IP/BP of the following drugs: sodium salicylate, calcium lactate, yellow mercuric oxide, ferrous fumarate, ferric ammonium citrate.

PART II

1. Assay of the following synthetic drugs: 1. Aspirin, 2. Paracetamol, 3. Sulphadiazine (or any other sulphonamide), 4. Isoniazid, 5. Benzyl benzoate, 6. Oxyphenbutazone.
2. Determination of Iodine value and Saponification value of fixed oil (Olive oil)
3. Colorimetric/Spectrophotometric determination of 1) Aniline 2) Glucose 3) Cholesterol 4) Ascorbic acid 5) Streptomycin, 6) Aspirin, 7) sulpha drug (Sulphadiazine, Sulphaguanidine).
4. Analysis of official drugs using common analytical techniques- Amperometric analysis of sulpha drugs
5. Assay of Vitamins: ascorbic acid, niacinamide, pyridoxine and thiamine.
6. Assay of some alkaloids official in IP/BP: atropine, codeine, ephedrine and quinine. Analysis of liquid extracts of some alkaloidal content.

PART III

Macroscopic examination, identification, description with constituents present and pharmacological action of crude drugs (15 common medicinal plants are to be studied).

PART IV- Viva voce

References

[1] A.O. Bentley, J.E. Driver, Bentley and Driver's Textbook of Pharmaceutical Chemistry, 7^{th} Edn., Oxford University Press, 1960.

[2] G.L. Genkins, A.M. Knevel, F.E. DiGangi, Quantitative Pharmaceutical Chemistry, 7^{th} 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

[6] M.A. Iyengar, Pharmacognosy of Crude Drugs.

[7] T.E.Wallis, Practical Pharmacognosy, Churchill, London, 1955.

PG4PHA P05 DRUG SYNTHESIS AND DISPENSING PRACTICAL

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

PART I Preparation of drug and drug intermediates.

I. Preparation Involving Multistep Synthetic Sequences

1. Benzaldehyde –Benzoin-benzyl.
2. Benzoin--Benzil-Dilantin
3. Phthalic acid-- Phthalic anhydride—phthalimide-- anthranilic acid
4. Flourescein---Dibromofluorescein---Mercurochrome
5. Methyl benzoate –methyl m-nitrobenzoate—m-nitrobenzoic acid
6. Aniline—acetanilide—p-nitroacetanilide
7. Acetanilide- 4-Acetamidobenzene sulphonyl chloride-4-Acetamido benzenesulfonamide-- Sulphanilamide

II. Preparation Involving Green Alternatives of Chemical Methods

1. Bisnaphthol from 2-naphthol
2. Coenzyme catalyzed benzoin condensation using thiamine hydrochloride
3. Photoreduction of benzophenone to benzopinacol using isopropanol
4. Benzopinacol to benzopinacolone
5. Acetanilide from aniline using zinc dust

III. Microwave assisted Organic Synthesis

1. 2-Hydroxychalcone from salicylaldehyde and acetophenone
2. 3-Methyl-1-phenyl-5-pyrazolone from ethyl acetoacetate
3. Benzoic acid from ethyl benzoate
4. Ethyl- 3-nitrobenzoate from 3- nitrobenzoic acid

PART II

Prediction of FTIR, ^{1}H and ^{13}C NMR spectra of the intermediates and products at each stage of synthesis by the above methods.

PART III 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. Mixtures: Typical mixtures involving incompatibilities.

PART IV- Viva voce

References

[1] A.I. Vogel, A Textbook of Practical Organic Chemistry, Longman, 1974.

[2] A.I. Vogel, Elementary Practical Organic Chemistry, Longman, 1958.

[3] F.G. Mann and B.C Saunders, Practical Organic Chemistry, 4th Edn., Pearson Education India, 2009.

[4] J.R. Adams, J.R. Johnson, J.F. Wilcox, Laboratory Experiments in Organic Chemistry, Macmillan, 1979.

[5] V.K. Ahluwalia, Green Chemistry: Environmentally Benign Reactions, Ane Books, 2009.

[6] Monograph on Green Chemistry Laboratory Experiments, Green Chemistry Task Force Committee, DST, 2009.

[7] R.M Silverstein, Spectrometric Identification of Organic compounds.

[8] F. G. Mann and B.C. Saunders, Practical Organic Chemistry, Pearson.

[9] J. B. Cohen, Practical Organic Chemistry, Mc Graw Hill.

[10] C.E Bella and DF Taber, Organic Chemistry Laboratory, Thomson.

[11] T. E. Wallis, Practical Pharmacognosy, Churchill, 1948.

[12] A.O. Bentley, J.E. Driver, Bentley and Driver's Textbook of Pharmaceutical Chemistry, 7th Edn., Oxford University Press, 1960.

[13] K.A. Connors, A Textbook of Pharmaceutical Analysis, John Wiley & Sons, 2007.

[14] J.W. Cooper, C. Gunn, Cooper and Gunn's Dispensing for Pharmaceutical Students, Pitman Medical, 1967.

[15] A. Kar, Advanced Practical Medicinal Chemistry, New Age International, 2007.

PG4PHA P06 BIOCHEMISTRY AND BACTERIOLOGY PRACTICAL

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

Biochemistry

PART I

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**

   Sample collection, Fixing of DO, Determination of refractive index, salinity, DO, BOD, COD, nitrite, sulphate, nitrate, phosphate, silicate analysis, Microbial analysis. Estimation of total dissolved matter, chloride, saline and albuminoid ammonia and COD.

PART II

1. Isolation of phytochemicals from their natural sources.
   1) Caffeine from Tea, 2) Nicotine from tobacco, 3) Curcumin from turmeric, 4) Tannins from Gallnuts 5) Lycopene from tomato.
2. Separations of mixtures by Paper Chromatography- 1) Separation of amino acids 2) Separation of dyes
3. Separation of serum proteins by paper electrophoresis.

Bacteriology

PART III

1) Preparation of some typical nutrient media for collection and isolation of bacteria.
2) Nutrient Agar, Endo's Agar, Chapman's Agar, Tergotol-7 Agar and McConkey Agar.
3) Staining and the study of the morphology of the bacteria.
4) Simple stain, b. Gram stain (Huker method), c. Negative stain (India ink method)
5) Fermentation test
6) Identification of some common pathogenic organisms.
7) Method of study of antibacterial activity of compounds and complexes.

PART IV- Viva voce

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, 5th Edn., 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.

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M.Sc. APPLIED CHEMISTRY

M.Sc. APPLIED CHEMISTRY

	Code	Course	Hours/ week	Total Hours	Credit	Marks		
						Internal	External	Total
Semester 1	PG1APL C01	Inorganic Chemistry-I (Coordination & Nuclear Chemistry)	4	72	4	20	80	100
	PG1APL C02	Organic Chemistry-I (Structure, Reactivity & Stereochemistry)	4	72	4	20	80	100
	PG1APL C03	Theoretical Chemistry-I (Quantum Chemistry and Group Theory)	4	72	4	20	80	100
	PG1APL C04	Physical chemistry- I (Kinetic Theory, Thermodynamics and Statistical Thermodynamics)	3	54	3	20	80	100
	PG2APL P01	Inorganic Chemistry Practical–1	3	54	Evaluation at the end of second semester			
	PG2APL P02	Organic Chemistry Practical-1	3	54				
	PG2APL P03	Physical Chemistry Practical -1	4	72				
		Total	**25**	**450**	**15**			
Semester 2	PG2APL C05	Inorganic Chemistry-II (Bioinorganic & Organometallic Chemistry)	4	72	4	20	80	100
	PG2APL C06	Organic Chemistry- II (Reaction Mechanism)	4	72	4	20	80	100
	PG2APL C07	Theoretical Chemistry – II (Chemical Bonding and Computational Chemistry)	4	72	4	20	80	100
	PG2APL C08	Physical chemistry- II (Molecular Spectroscopy)	3	54	3	20	80	100
	PG2APL P01	Inorganic Chemistry Practical–1	3	54	3	20	80	100
	PG2APL P02	Organic Chemistry Practical-1	3	54	3	20	80	100
	PG2APL P03	Physical Chemistry Practical -1	4	72	4	20	80	100
		Total	**25**	**450**	**25**			

Semester 3	PG3APL C09	Organic Chemistry- III (Advanced Synthetic Organic Chemistry)	4	72	4	20	80	100
	PG3APL C10	Physical chemistry- III (Selected topics in Physical Chemistry)	4	72	4	20	80	100
	PG3APL C11	Fatty acids, Nano and Green chemistry	4	72	4	20	80	100
	PG3APL C12	Spectroscopic methods in Chemistry	3	54	3	20	80	100
	PG4APL P04	Industrial oil and fat products Practical	3	54	Evaluation at the end of fourth semester			
	PG4APL P05	Essential oil and aromatics Practical	3	54				
	PG4APL P06	Fixed oils and fats Practical	4	72				
		Total	**25**	**450**	**15**			
Semester 4	PG4APL E01	Elective 1 Analysis of Fats, Oils and Waxes	5	90	4	20	80	100
	PG4APL E02	Elective 2 Industrial Oil and Fat Products	5	90	4	20	80	100
	PG4APL E03	Elective 3 Essential Oils and Aromatics	5	90	4	20	80	100
	PG4APL E04	Elective 4 Polymer Chemistry	5	90	4	20	80	100
	PG4APL E05	Elective 5 Analytical Chemistry	5	90	4	20	80	100
	PG4APL P04	Industrial Oil and Fat Products Practical	3	54	3	20	80	100
	PG4APL P05	Essential Oils and Aromatics Practical	3	54	3	20	80	100
	PG4APL P06	Fixed Oils and Fats Practical	4	72	3	20	80	100
	PG4APL D01	Project			2	20	80	100
	PG4APL V01	Viva			2	20	80	100
		Total	**25**	**450**	**25**			
Grand Total					**80**			

SEMESTER 1

PG1APL C01 INORGANIC CHEMISTRY – I

(COORDINATION & NUCLEAR CHEMISTRY)

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

Module 1: Coordination Chemistry- Structural Aspects and Bonding (18 Hrs)

1.1 Classification of complexes based on coordination numbers and possible geometries. σ and π bonding ligands such as CO, NO, CN^-, R_3P and Ar_3P.

1.2 Splitting of *d* orbitals in octahedral, tetrahedral, square planar, square pyramidal and trigonal 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 with and without π-bonding, experimental evidences for π-bonding

Module 2: Kinetics and Mechanism of Reactions in Metal Complexes (18 Hrs)

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

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

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

Module 3: Organometallic Compounds- Synthesis, Structure and Bonding (18 Hrs)

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

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

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

Module 4: Electron deficient compounds (9 Hrs)

Electron deficient compounds – synthesis, reactions, structure and bonding. Boron hydrides, styx numbers, Boron cluster compounds.

Wade's rule, Hydroborate anions, Organoboranes and hydroboration, Polyhedral anions, Carboranes, Metalloboranes, Borazines and Borides.

Module 5: Nuclear Chemistry (9 Hrs)

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

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

5.3 Analytical applications of radioisotopes- radiometric titrations, kinetics of exchange reactions, measurement of physical constants including diffusion constants, neutron activation analysis, prompt gamma neutron activation analysis and neutron absorptiometry.

5.4 Applications of radio isotopes in industry, medicine, autoradiography, radiopharmacology, radiation safety precaution, nuclear waste disposal.

5.5 Radiation chemistry of water and aqueous solutions- Fricke solution, Ceric ammonium solution. Measurement of radiation doses. Relevance of radiation chemistry in biology, organic compounds and radiation polymerization.

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PG1APL C02 ORGANIC CHEMISTRY - I

(STRUCTURE, REACTIVITY & STEREOCHEMISTRY)

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

Module 1: MO Theory and Aromaticity (9 Hrs)

1.1 Review of basic concepts in organic chemistry: bonding, hybridization, MO picture (allyl system, 1,3-butadiene and benzene), inductive effect, electromeric effect, resonance effect, hyperconjugation, steric effect. Bonding weaker than covalent bonds.

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

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

Module 2: Investigation of Organic Reaction Mechanisms (9 Hrs)

Energy profiles, Methods of determining reaction mechanisms, Kinetic and thermodynamic control of reactions. The Hammond postulate. Principle of microscopic reversibility. Marcus theory. The Hammett equation and its applications. Taft equation. Linear free energy relationships. Solvent polarity and parameters. Y, Z and E parameters and their applications. Primary and secondary kinetic isotope effects. Salt effects and special salt effects in SN reactions. Solvent effect. Bulk and specific solvent effects. Introduction to carbon acids - pKa of weak acids, kinetic and thermodynamic acidity. Phase transfer catalysis and its applications. Steric effects. HSAB principle and its applications in organic reactions.

Module 3: Review of Organic Reaction Mechanisms (18 Hrs)

3.1 Review of organic reaction mechanisms with special reference to nucleophilic and electrophilic substitution at aliphatic carbon (S_N1, S_N2, S_Ni, S_E1, S_E2, addition-elimination and elimination-addition sequences), elimination (E1 and E2). Elimination vs substitution.

3.2 A comprehensive study on the effect of substrate, reagent, leaving group, solvent and neighbouring group on nucleophilic substitution (S_N2 and S_N1) and elimination (E1 and E2) reactions.

3.3 Addition reactions (regioselectivity- Markovnikov's addition- carbocation mechanism, anti-Markovnikov's addition- radical mechanism).

3.4 Mechanism of electrophilic and nucleophilic aromatic substitution reactions with examples. Arenium ion intermediates. S_N1, S_NAr, $S_{RN}1$ and Benzyne mechanisms.

3.5 Catalysis by acids, bases and nucleophiles with examples from acetal, cyanhydrin and ester formation and hydrolysis reactions- $A_{AC}2$, $A_{AC}1$, $A_{AL}1$, $B_{AC}2$ and $B_{AL}1$ mechanisms.

Module 4: Stereochemistry of Organic Compounds (18 Hrs)

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

4.2 Stereoisomerism: Definition based on symmetry and energy criteria, configurational and conformational stereoisomers.

4.3 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 C_n, molecules with more than one center of chirality, definition of diastereoisomers, constitutionally symmetrical and unsymmetrical chiral molecules, erythro and threo nomenclature.

4.4 Axial, planar and helical chirality with examples, stereochemistry and absolute configuration of allenes, biphenyls, binaphthyls, ansa and cyclophanic compounds, spiranes, exocyclic alkylidene cycloalkanes.

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

4.6 Geometrical isomerism: Nomenclature, E-Z notation, methods of determination of geometrical isomers. Interconversion of geometrical isomers.

Module 5: Conformational Analysis (18 Hrs)

5.1 Conformational descriptors- factors affecting conformational stability of molecules. Conformational analysis of acyclic and cyclic systems: substituted ethanes, cyclohexane and its derivatives, decalins, adamantane, congressane, sucrose and lactose. Fused and bridged bicyclic systems.

5.2 Conformation and reactivity of elimination (dehalogenation, dehydrohalogenation, semipinacolic deamination and pyrolytic elimination- Saytzeff and Hofmann eliminations), substitution and oxidation of 2° alcohols. Chemical consequence of conformational equilibrium - Curtin Hammett principle. Chiral drugs.

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[1] R. Bruckner, Advanced Organic Chemistry: Reaction Mechanisms, Academic Press, 2002.

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PG1APL C03 THEORETICAL CHEMISTRY – I

(QUANTUM CHEMISTRY AND GROUP THEORY)

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

Module 1: Formulation of Quantum Chemistry (18 Hrs)

1.1 Mathematical Concepts (5 Hrs)

Co-ordinate systems: Cartesian, Cylindrical polar and Spherical polar coordinates and their relationships. Complex numbers: definition, Complex conjugate, absolute value of a complex number, complex functions. Operator algebra: linear and nonlinear operators, Hermitian operators, del and del-squared operators. Eigen function and eigen values of an operator, Eigen value equation, Eigen functions of Commuting operators. Well behaved functions, Normalized and Orthogonal functions.

1.2 Evolution of Quantum Mechanics (5 Hrs)

Failure of classical mechanics: The black body radiation, Compton effect, photoelectric effect, atomic spectra. Need of quantum mechanics. Concept of matter wave, de Broglie relation and its experimental proof, Uncertainty principle and its consequences. Wave function and Born interpretation, Schrödinger's wave mechanics, Deduction of Schrodinger equation from classical wave equation.

1.3 Postulates of Quantum Mechanics (4 Hrs)

Detailed discussion of postulates: State function postulate. Operator postulate. Eigen value postulate. Expectation value postulate. Postulate of time dependent Schrodinger equation of motion, Conservative system and time-independent Schrodinger equation.

1.4 Quantum Mechanics of Translational Motion (4 Hrs)

Particle in one-dimension with infinite potential walls, particle in a three dimensional box- separation of variables- rectangular box and cubic box, degeneracy. Introduction to tunnelling with experimental evidence.

Module 2: Applications of Quantum Chemistry (18 Hrs)

2.1 Quantum Mechanics of Hydrogen-like Atoms (5 Hrs)

Potential energy of hydrogen-like systems. The wave equation in spherical polar

coordinates: separation of variables- R, Θ and Φ equations and their solutions, wave functions and energies of hydrogen-like atoms. Orbitals- radial functions, radial distribution functions, angular functions and their plots.

2.2 Quantum Mechanics of Vibrational Motion (5 Hrs)

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. Rodrigue's formula, Three dimensional harmonic oscillator.

2.3 Quantum Mechanics of Rotational Motion (5 Hrs)

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 Φ equation and its solution, wave functions in the real form. Non-planar rigid rotor (or particle on a sphere)- separation of variables, the Φ and the Θ equations and their solutions, Legendre and associated Legendre equations, Legendre and associated Legendre polynomials. Spherical harmonics (imaginary and real forms)- polar diagrams of spherical harmonics.

2.4 Orbital and Spin angular momentum (3 Hrs)

Quantisation of angular momentum, quantum mechanical operators corresponding to angular momenta, (L_x, L_y, L_z and L^2). Commutation relations between these operators. Spherical harmonics as eigen functions of angular momentum operators L_z and L^2. Space quantization. The postulate of spin by Uhlenbeck and Goudsmith, discovery of spin- Stern Gerlach experiment. Spin orbitals- construction of spin orbitals from orbital and spin functions.

Module 3: Molecular Symmetry and Mathematical group (18 Hrs)

3.1 Symmetry elements and symmetry operations. Conditions for a set of elements to form a group, sub groups, abelian and cyclic groups, Point groups. Multiplication of operations. Group multiplication table of C_{2v}, C_{2h} and C_{3v} groups (H_2O, Trans N_2F_2 and NH_3 as examples). Similarity transformation and classes in a group.

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

3.3 Reducible and Irreducible representations (IR). Reduction formula, reduction of reducible representation to IRs.

Module 4: Applications of Group Theory (18 Hrs)

4.1 The Great Orthogonality theorem. Rules derived from GOT (proof not required). Setting up of character table of C_{2v}, C_{3v}, C_{2h}, C_{4v} and C_3 groups. Direct product representations.

4.2 Applications in quantum mechanics, transition moment integral, vanishing of integrals. Jahn – Teller effect, Woodward – Hoffmann rules.

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

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

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PG1APL C04 - PHYSICAL CHEMISTRY - II

(KINETIC THEORY, THERMODYNAMICS AND STATISTICAL THERMODYNAMICS)

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

Module 1: Kinetic theory **(9 Hrs)**

Kinetic theory of gases, 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, transport properties of gases. Viscosity, thermal conductivity and diffusion. Determination of viscosity of gases. Influence of temperature and pressure on transport properties.

Module 2: Classical Thermodynamics **(18 Hrs)**

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

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

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

2.4 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.

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

2.6 Chemical affinity and thermodynamic functions, effect of temperature and pressure on chemical equilibrium- van't Hoff reaction isochore and isotherm.

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

2.8 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, and three pairs of partially miscible liquids.

Module 3: Irreversible Thermodynamics and Bioenergetics (9 Hrs)

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

Module 4: Statistical Thermodynamics (18 Hrs)

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

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

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[1] P.W. Atkins, Physical Chemistry, ELBS, 1994.

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SEMESTER 2

PG2APL C05 INORGANIC CHEMISTRY- II

(BIOINORGANIC & ORGANOMETALLIC CHEMISTRY)

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

Module 1: Acids, Bases and Non-aqueous solvents (9 Hrs)

1.1 Acid base concept in non-aqueous media-HSAB concept, solvent effect, linear free energy relationship- mechanism and method of determination.

1.2 Reaction in non-aqueous solvents. Ammonia- solution of metals in liquid ammonia. Protonic solvents: anhydrous sulphuric acid, hydrogen halide. Aprotic solvents: non-polar solvents, non-ionizable polar solvents. Polar solvents undergoing autoionization. Liquid halogen, Inter halogen compounds, oxy halides, dinitrogen tetroxide, sulphur dioxide.

Module 2: Bioinorganic Compounds (18 Hrs)

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

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

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

Module 3: Spectral and Magnetic Properties of Metal Complexes (18 Hrs)

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

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

3.3 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.

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

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

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

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

Module 5: Stereochemistry of Coordination Compounds (9 Hrs)

5.1 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.

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

Module 6: Reactions of Organometallic Compounds (9 Hrs)

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

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

6.3 Rearrangement reactions, redistribution reactions, fluxional isomerism.

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

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

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PG2APL C06 ORGANIC CHEMISTRY - II

(REACTION MECHANISM)

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

Module 1: Chemistry of Carbocations (9 Hrs)

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

1.2 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, Demjanov rearrangement. Oxymercuration, halolactonisation.

Module 2: Chemistry of Carbanions (18 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, Kinetic and thermodynamic enolates- Lithium and boron enolates in Michael and aldol reactions, alkylation and acylation of enolates. Chemistry of enamines, Stork-Enamine reaction.

2.2 Nucleophilic additions to carbonyls groups. Reactions involving carbanions-mechanisms of Claisen, Dieckmann, Knoevenagel, Stobbe, Darzen and acyloin condensations, Shapiro reaction and Julia elimination. Favorskii rearrangement.

2.3 Reactions of carbonyl compounds: oxidation, reduction (Clemmensen and Wolff-Kishner), addition reactions (addition of cyanide, ammonia, alcohol), Aldol condensation, Cannizzaro reaction, addition of Grignard reagent.

2.4 Structure and reactions of α, β- unsaturated carbonyl compounds involving electrophilic and nucleophilic addition- Michael addition, Mannich reaction, Robinson annulation.

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

Module 3: Carbenes, Carbenoids, Nitrenes and Arynes (9 Hrs)

3.1 Generation, structure and reactions of carbenes. Rearrangement reactions of carbenes: Wolff rearrangement, generation and reactions of ylids by carbenoid decomposition.

3.2 Structure, generation and reactions of nitrenes. Hoffmann, Curtius, Lossen, Schmidt and Beckmann rearrangement reactions.

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

Module 4: Radical Reactions (9 Hrs)

4.1 Generation and detection 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. Autoxidation.

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

Module 5: Concerted reactions (18 Hrs)

5.1 Symmetry properties of molecular orbitals of ethylene and conjugated systems with three or more atoms, Woodward – Hoffmann rule, Conservation of orbital symmetry and stereo chemical courses.

5.2 Pericyclic reactions like Electrocyclic (butadiene-cyclobutene and hexatriene-cyclohexadiene interconversions), Cycloadditions (2+2) & (4+2), Sigmatropic (1,3), (1,5) and (3,3), Cheletropic including Cheletropic eliminations and Ene reaction with stereo chemical aspects.

5.3 Diels- Alder reactions with stereochemical aspects.

5.4 Analysis of Pericyclic Reactions. (i) FMO method (ii) Orbital- correlation method and (iii) PMO method.

5.2 Highlighting pericyclic reactions in organic synthesis such as Claisen, Cope, Mislow-Evans, Wittig and Sommelet-Hauser rearrangements. dipolar cycloaddition (introductory). Unimolecular pyrolytic elimination reactions, decomposition of

cyclic azo compounds, β-eliminations involving cyclic transition states such as N-oxides, acetates and xanthates.

Module 6: Organic Photochemistry **(9 Hrs)**

6.1 Photochemical processes. Energy transfer. Jablonski diagram, sensitization and quenching. Singlet and triplet states and their reactivity.

6.2 Photoreactions of carbonyl compounds, enes, dienes and arenes. Norrish reactions of acyclic ketones. Patterno-Buchi, Barton, Photo-Fries and Di-л methane rearrangements. Photoreactions of Vitamin D. Photosynthesis and photochemistry of vision. Singlet oxygen generation and their reactions.

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[1] R. Bruckner, Advanced Organic Chemistry: Reaction Mechanism, Academic Press, 2002.

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PG2APL C07 THEORETICAL CHEMISTRY - II

(CHEMICAL BONDING AND COMPUTATIONAL CHEMISTRY)

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

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

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

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

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

Module 2: Chemical Bonding (18 Hrs)

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

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

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

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

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

Module 4: Computational Chemistry (18 Hrs)

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

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

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

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

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

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

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

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

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

Module 5: Computational Chemistry Calculations (9 Hrs)

5.1 Molecular geometry input- Cartesian coordinates and internal coordinates, Z-matrix. Z-matrix of: single atom, diatomic molecule, non-linear triatomic molecule, linear triatomic molecule, polyatomic molecules like ammonia, methane, ethane and butane. General format of GAMESS/Firefly input file. GAMESS/Firefly key word for: basis set selection, method selection, charge, multiplicity, single point energy calculation, geometry optimization, constrained optimization and frequency calculation.

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

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

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Softwares

Molecular Mechanics:

01. **Arguslab** available from www.arguslab.com/
02. **Tinker** available from www.dasher.wustl.edu/ffe/

Ab initio, semiempirical and dft:

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

Graphical User Interface (GUI):

01. **Gabedit** available from http://gabedit.sourceforge.net/
02. **wxMacMolPlt** available from http://www.scl.ameslab.gov/MacMolPlt/
03. **Avogadro** from http://avogadro.openmolecules.net/wiki/Get_Avogadro

PG2APL C08 PHYSICAL CHEMISTRY - II

(MOLECULAR SPECTROSCOPY)

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

Module 1: Microwave and Infrared Spectroscopy (18 Hrs)

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

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

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

Module 2: Electronic, Mossbauer and Raman spectroscopy (18 Hrs)

2.1 Electronic spectroscopy: Term symbols of diatomic molecules, electronic spectra of diatomic molecules, selection rules, vibrational coarse structure and rotational fine structure of electronic spectrum, Franck-Condon principle, predissociation, calculation of heat of dissociation, Birge and Sponer method, electronic spectra of polyatomic molecules, spectra of transitions localized in a bond or group, free electron model.

Different types of lasers- solid state lasers, continuous wave lasers, gas lasers and chemical laser, frequency doubling, applications of lasers, introduction to UV and X-ray photoelectron spectroscopy.

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

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

Module 3: Resonance Spectroscopy (18 Hrs)

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

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

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

3.4 An elementary study of NQR spectroscopy.

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

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SEMESTERS 1 AND 2

PG2APL P01 INORGANIC CHEMISTRY PRACTICAL – 1

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

PART I

Separation and identification of four metal ions of which two are rare/ less familiar such as Tl, W, V, Se, Te, Ti, Ce, Th, Zr, U, Mo and Li and common cations - 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+}, Co^{2+}, Ni^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}, Mg^{2+}, Li^{+}, Na^{+}, K^{+}, NH_4^{+} (interfering acid radicals are not present). Confirmation by spot test (Minimum **8** mixtures are to be recorded).

PART II

1. Argentometric estimation of chlorides
2. Cerimetry – Fe(II) and nitrate
3. Potassium iodate – iodide estimation of Sn(II)

PART III

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

PART IV

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

1. Tris (thiourea) copper (I) complex
2. Potassium tris (oxalate) aluminate (III)
3. Tetrammine copper (II) sulphate
4. Mercury tetra thiocyanato cobaltate (III)

References

[1] A.I. Vogel, A Text Book of Qualitative Inorganic Analysis Including Elementary Instrumental Analysis, 3rd Edn., ELBS.

[2] G. Svelha, Text Book of Vogel's Macro and Semi-micro Inorganic Analysis, revised, Orient Longman.

[3] V.V. Ramanujam, Inorganic Semi micro Qualitative Analysis, The National Publishing Co., Chennai.

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

PG2APL P02 ORGANIC CHEMISTRY PRACTICAL - 1

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

PART I

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

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

PART II

A. Separation of organic binary mixtures:- 1. Quantitative separation of a mixture oftwo components by solvent extraction 2. Purification of the separated samples by distilling and crystallization. 3. Determination of physical constants of separated and purified samples (No need of bifunctional compounds).

B. Separation of organic mixtures by TLC and calculation of R_f values.

C. Separation/purification of organic mixtures by column chromatography.

PART III

Drawing the structures of organic molecules and reaction schemes and mechanisms by ChemDraw, SymyxDraw and Chemsketch.

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

PART IV- Viva voce

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PG2APL P03 PHYSICAL CHEMISTRY PRACTICAL - 1

Credit: 4 **Contact Lab Hours: 72+72 =144**

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

Part A

I. Adsorption

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

II. Phase diagrams

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

III. Distribution law

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

IV. Surface tension

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

Part B

Computational Chemistry Experiments

V. Experiments illustrating the capabilities of modern open source/free computational chemistry packages in computing single point energy, geometry optimization, vibrational frequencies, population analysis, conformational studies, IR and Raman spectra, transition state search, molecular orbitals, dipole moments etc.
Geometry input using Z-matrix for simple systems, obtaining Cartesian coordinates from structure drawing programs like Chemsketch.

References

[1] J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.
[2] G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8^{th} Edn., McGraw Hill, 2009.
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SEMESTER 3

PG3APL C09 – ORGANIC CHEMISTRY- III
(ADVANCED SYNTHETIC ORGANIC CHEMISTRY)

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

Module 1: Retrosynthetic Analysis (9 Hrs)

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

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

Module 2: Organic Synthesis via Oxidation and Reduction (18 Hrs)

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

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

Module 3: Modern Synthetic Methods and Reagents (9 Hrs)

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

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

Module 4: Stereoselective Transformations (9 Hrs)

4.1 Assymmetric induction, chiral auxiliaries and chiral pool.

4.2 Enatioselective catalytic hydrogenation developed by Noyori and Knowels.

4.3 Assymetric aldol condensation pioneered by Evans.

4.4 Assymmetric Diels Alder reactions.

4.5 Assymmetric epoxidation using Jacobsen's catalyst.

Module 5: Construction of Carbocyclic and Heterocyclic Ring Systems (9 Hrs)

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

5.2 Formation of heterocyclic rings: 5- and 6-membered and condensed ring heterocyclic compounds with one or more than one hetero atom like N, S or O - pyrrole, furan, thiophene, pyridine, imidazole, thiazole, oxazole, pyrimidines, purines, quinoline and isoquinoline.

Module 6: Molecular Recognition and Supramolecular Chemistry (9 Hrs)

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

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

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

6.4 Applications of supramolecular complexes in medicine and perfumery industries.

Module 7: Chemistry of Natural products and Biomolecules (9 Hrs)

7.1 Basic aspects of structure and classification of carbohydrates, alkaloids, steroids, plant pigments, vitamins, amino acids, proteins and nucleic acids (Structure elucidation of papaverine and quinine only).

7.2 Methods for primary structure determination of peptides, proteins and nucleic acids. 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).

References

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[18] E. J. Corey, Xue-Min Cheng, The Logic of Chemical Synthesis, Wiley, 1995.

[19] J. Zhu, Q. Wang, M. Wang (Eds), Multicomponent Reactions in Organic Synthesis, Wiley VCH, 2015

[20] F. Rutjes, V.V. Fokin, K.B. Sharpless, Click Chemistry: In Chemistry, Biology and Macromolecular Science, Wiley, 2012.

PG3APL C10- PHYSICAL CHEMISTRY- III
(SELECTED TOPICS IN PHYSICAL CHEMISTRY)

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

Module 1: Quantum Statistics (9 Hrs)

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

1.2 Heat capacity of solids- Dulong and Petit's law, the vibrational properties of solids, Einsteins theory- derivation and its limitations, Debye theory – derivation and its limitations.

Module 2: Chemical Kinetics (18 Hrs)

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

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

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

Module 3: Catalysis **(9 Hrs)**

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

3.2 Enzyme catalysis and its mechanism, Michaelis-Menton equation, effect of pH and temperature on enzyme catalysis.

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

Module 4: Surface Chemistry **(18 Hrs)**

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

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

4.3 Vacancy theory of liquids, free volume of a liquid, physical properties of liquids-surface tension, determination of surface tension, optical activity and molar refraction.

Module 5: Colloids **(18 Hrs)**

5.1 Colloidal systems, classification, preparation of colloidal solution, purification of colloidal solution, properties of colloidal systems- electrical properties, electrical double layer, Zeta potential, electrokinetic phenomena, sedimentation potential and streaming potential, electrophoresis, electroosmosis, Donnan membrane equilibrium, coagulation of colloidal solutions, determination of size of colloidal particles, micelle formation, critical micelle concentration, factors affecting CMC in aqueous media , location of solubilizates in micelles, phase rule of solubilization.

5.2 Emulsification, macroemulsions, factors determining stability of emulsion, microemulsion, theories of emulsions, selection of surfactants as emulsifying agents, Gels and their preparation, importance and applications of colloids.

5.3 Macromolecules: different averages, relation between different averages, calculation of different averages.

References

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

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PG3APL C11 FATTY ACIDS, NANO AND GREEN CHEMISTRY

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

Module 1: Lipids **(9 Hrs)**

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

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

1.3 Nomenclature of fatty acids- IUPAC and omega reference systems, Polymorphism of fats and fatty acids. Chemical synthesis of fatty acids and their derivatives, uses of fatty acids in textiles, leather, pharmaceuticals and petroleum processing.

Module 2: Isolation and Characterization of Fatty Acids **(9 Hrs)**

2.1 Crystallisation methods, advanced methods of analysis of oils: Harmonization of standard methods. Chromatography of oils, fats and derivatives. Packed column gas chromatography, WCOT (capillary) and SCOT GLC, Thin layer and paper chromatography, High performance liquid chromatography, Applications of semi-permeable membranes in the analysis of oils and allied products. Applications of TLC-FID. Stereospecific analysis of triacylglycerols.

2.2 Use of IR, UV, NMR and mass spectrometry, GC-FID, Fragmentation pattern – special reference to stearates and oleates, Application of wide line NMR in the oils and fats industry.

Module 3: Fatty Acids Occurring in Nature **(9Hrs)**

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

3.2 Unsaturated fatty acids: monoethenoid fatty acids-their occurrence and general methods of synthesis. Oleic acid and petroselenic acid- properties and constitution, other monoethenoid acids occurring in animal and vegetable oils and fats.

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

Module 4: Properties of Fatty Acids (18 Hrs)

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

4.2 Salt formation, esterification, halogenation, oxidation, uses of various oxidizing agents like chromic acid, ozone, peroxides, potassium permanganate, periodic acid and lead tetra acetate. Hydrogenation, dehydration, pyrolysis, polymerization, addition reactions to double bond. Rancidity in oils, fats and oil bearing substances, tests for rancidity, stability of oils, induction period, pro-oxidants and antioxidants, drying, semidrying and nondrying oils. Concept of autoxidation, theories of autoxidation Biointer-esterification: Chemistry and technology of biointer-esterification, Detection of inter esterified fats. Application of Bio-inter esterification.

Module 5: Biochemistry and Metabolism of Fats (9 Hrs)

5.1 Essential fatty acids. Biosynthesis of fatty acids, Biochemical transformation of fats in the body, biosynthesis of fats in plants and animal organisms.

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

Module 6: Nanotechnology and Its Innovations in Chemical Industry (9 Hrs)

6.1 Introduction to Nanomaterials, Types of Nanomaterials: Fullerenes, Carbon Nanotubes, Nanowires, Nanocones, Haeckelites, Quantum dots and Graphenes.

6.2 Brownian Motion, Surface Forces, Self Assembly, Top-down Production, Bottom-up Production.

6.3 Innovations of Nanotechnology in: Refineries, Production of Biofuel, Edible Oils, Cosmetics, Food and Packaging Industry, Pharmaceuticals, Textiles, Polymers, Paints and Dyes. General Applications.

Module 7: Green Chemistry **(9 Hrs)**

7.1 Principles of green chemistry, atom economy, principles of green organic synthesis, green alternatives of organic synthesis-coenzyme catalysed reactions, green alternatives of molecular rearrangements, electrophilic aromatic substitution reactions, oxidation-reduction reactions, clay catalysed synthesis, condensation reactions, Green photochemical reactions.

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

7.3 General principles of microwave assisted organic synthesis.

References

[1] M.G. Wohl, R.S. Goodhart, M.E. Shils, Modern Nutrition in Health and Disease, 6th Edn., Lea & Febiger, 1980.

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[14] E. H. Pryde, Natural fatty acids and their sources.

[15] H. Patterson, Hydrogenation of fats and oils, Applied Science Publishers, 1983.

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PG3APL C12 SPECTROSCOPIC METHODS IN CHEMISTRY

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

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

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

1.2 Influence of substituent, ring size and strain on spectral characteristics. Solvent effect, Stereochemical effect, non-conjugated interactions.

1.3 Problems based on the above topics.

1.4 Chirooptical properties- ORD, CD, octant rule, axial haloketone rule, Cotton effect.

Module 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.

Module 3: Nuclear Magnetic Resonance Spectroscopy (18 Hrs)

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

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

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

3.4 2D NMR and COSY, HOMOCOSY and HETEROCOSY

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

3.6 Problems on spectral interpretation with examples.

Module 4: Mass Spectrometry (9 Hrs)

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

4.2 Problems on spectral interpretation with examples.

Module 5: Structure Elucidation Using Spectroscopic Techniques (9 Hrs)

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

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

References

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

[2] A.U. Rahman, M.I. Choudhary, Solving Problems with NMR Spectroscopy, Academic Press, 1996.

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

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SEMESTER 4

ELECTIVE COURSES

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

PG4APL E01- ANALYSIS OF FATS, OILS AND WAXES

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

Module 1: Extraction of oils and fats (9 Hrs)

Mechanical pretreatment and heat treatment of oil bearing materials. Rendering of animal fats and cooking of oil seeds. Mechanical expression of oils. Solvent extraction-theory and practice, type of extractors, solvent recovery, alternative solvents for extraction, super critical fluid extraction of oils and fats. Newer methods in extraction of oils. Technical refining of oils for industrial uses, detoxification and technical products from oil cakes, edible products from oil meals, synthetic fatty material. Anti nutritional constituents of oil seeds. General methods of upgrading and utilization of oils, oil cakes and other products. Liquid-liquid extraction- distribution laws, use of oxine, dithiazone, high molecular weight amines, dithiocarbamates and crown ethers in extraction.

Module 2: Commercially important oils and fats (18 Hrs)

Study of the sources, composition, characteristics and utilization of commercially important oils and fats-butter, tallow, lard, coconut oil, palm oil, palm kernel oil, peanut oil, cocoa butter, olive oil, cotton seed oil, rice bran oil, sesame oil, soyabean oil, sunflower oil, tung oil, linseed oil, mustard oil, castor oil, hydnocarpus oil, marine oils. Specific methods for the production of palm oil, palm kernel oil and rice bran oil, jujoba oil and coconut oil.

Module 3: Oils and fats as food materials (9 Hrs)

3.1 Cooking oil, salad oil, and salad dressings. Quality evaluation of cooking oils and salad oils. Margarine and Shortenings, Production of plastic fats, Cocoa butter substitute, Food emulsions, Medicinal applications. Preparation of polyol and other esters.

3.2 Essential fatty acids: ω-3 and ω-6 fatty acids and their dietary sources, significance to human nutrition and health, thermal changes in oils, trans fatty acids, significance of unsaturated fatty acids in food.

Module 4: Glyceride structure **(9 Hrs)**

4.1 Glyceride composition of natural fats. Methods of investigation of glycerides. Theories of glyceride structure, Fatty acids, theory and practice of fat splitting and purification of products.

4.2 Glycerine: Processes for treatment of sweet water and spent soap lye, Manufacture of glycerine from natural sources. Synthetic glycerine, grades of glycerine, properties and utilization of glycerine. Advanced theories of glyceride structure of natural fats, determination of glyceride structure; synthesis of glycerides; estimation of mono-, di-, and tri-glycerides. Stereo-specific analysis, lipase hydrolysis.

4.3 Products obtained by inter esterification, hydrogenation, oxidation and pyrolysis. Metallic soaps.

Module 5: Analysis of fats and oils **(18 Hrs)**

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

5.2 Test methods for chemical properties: Iodine value, thiocyanogen number, saponification value, acid value and free fatty acid, oxirane oxygen, hydroxyl and acetyl value, peroxide value, Reichert-Meissl value, Polenski value and Kirschner value, diene value. Estimation of poly unsaturated fatty acids- Kries test, thiobarbituric acid test. Theory of the analysis of milk, butter, other diary items, starch based food products and beverages.

5.3 Adulteration of oils and fats – detection of adulteration. Food adulteration – common adulterants in food and their determination. Pesticide analysis in food products. Extraction and estimation of chlorinated pesticides in food products.

Module 6: Nonglyceride constituents of fats and oils (9 Hrs)

Occurrence, chemistry and function of carotenes, vitamins, tocopherols, steroids, phenolic compounds, phospholipids, sphingolipids, antioxidants. Constituents contributing flavour and odor.

Module 7: Waxes, fatty alcohols and drying oils (18 Hrs)

7.1 Occurrence, classification, properties and composition of waxes. Synthetic waxes. Analysis and utilization of waxes, wax content of vegetable oils.

7.2 Naturally occurring fatty alcohols-production- natural and petrochemical sources, common names and related compounds, nutritional aspects and applications. Fatty alcohols and amines: Methods of production and their utilization. Manufacture of sulphited and sulphurised oils, properties, specifications and plant and processes employed. Textile auxiliaries, leather chemicals, polymer additives, paint additives, lubricant additives, alcohol ethers.

7.3 Special quality control methods applied to oils, fats and allied industry - nickel content of hydrogenated oils; iron and phosphatide content of crude and refined vegetable oils.

7.4 Chemistry of drying oils: Modification of oils for surface coating industry. Thermal and chemical modification methods; properties of modified oils, changes in drying oils during heat bodying and oxidative polymerization. Malenised oils, epoxidised oils, boiled oils, blown oils, stand oils, urethane oils.

References

[1] D. Swern, Bailey's Industrial oil and Fat Products, Vol. I-II, 4th Edn., John Wiley & Sons, 1982.

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PG4APL E02 INDUSTRIAL OIL AND FAT PRODUCTS

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

Module 1: Processing of fats and oils (9 Hrs)

Processes and plants employed for refining, bleaching, deodorization, hydrogenation and winterization, stabilization, solidification, homogenization, emulsification and dewaxing of oils. Manufacture and evaluation of auxiliary materials such as activated earth and carbon, Ni catalyst and hydrogen. Newer techniques of refining of oils and fats. Manufacture of butter, margarine, ghee, vanaspati, bakery and confectionery fats and fatty foods. Composition and properties of the spoilage during storage of fats and fat products, protection against autoxidation.

Module 2: Hydrogenation of Oils (9 Hrs)

2.1 Catalytic hydrogenation: chemistry of hydrogenation, hydrogenolysis, influence of various factors in hydrogenation, mechanism, kinetics and thermodynamics of hydrogenation reactions, hydrogenation catalysts-theory of catalysis, materials and apparatus, new developments in plants and processes for hydrogenation.

2.2 Industrial processes of a) Manufacture of catalyst for hydrogenation, hydrogen production and purification. b) Hydrogenation of vegetable and marine oils-manufacture of vanaspati. c) Reduction of long chain fatty acids.

Module 3: Fat Splitting and Esterification (9Hrs)

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

3.2 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.

Module 4: Grease and Lubricating oil (9 Hrs)

4.1 Introduction to lubricants, liquid, solid and gas lubricants and their applications. Lubricating oils, liquid mineral lubricants, synthetic liquid lubricants. Physical properties, additives, manufacture of lubricating oils. Analysis of lubricating oils.

4.2 Lubricating Greases: Properties, types, ingredients, additives, analysis of lubricating greases as per BIS test methods. Manufacture of lubricating greases- Processes and equipments.

Module 5: Soaps and shampoos (9 Hrs)

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

5.2 Chemical analysis of soaps- T.F.M value of soaps, Cleansing action, Composition of shaving creams.

5.3 Shampoos: Ingredients and functions. Different kinds of shampoos. Anti-dandruff, anti-lice, herbal and baby shampoos. Health effects of shampoos.

Module 6: Synthetic Detergents (9 Hrs)

6.1 Detailed study of the chemistry and applications of anionic, cationic, amphoteric and nonionic detergents used in modern industries and for household purposes. Dish washes, neutral soaps, manufacture and applications. Agglomeration.

6.2 Merits and demerits of syndets over soaps, biodegradability of detergents.

6.3 Role of surfactants in synthesis of nanoparticles, enzyme detergents, green detergents and compact detergents.

Module 7: Paints, Varnishes and Lacquers (9 Hrs)

7.1 Paints as protective coatings, paints and enamels, materials for paint manufacture, oils used- unmodified oils and their pretreatment, modified drying oils, resins and copolymers- natural resins, phenolic resins, alkyd resins, urethane resins and epoxy resins.

7.2 Driers, thinners, pigments and miscellaneous ingredients, mechanism of polymerization and drying of oils.

7.3 Testing and evaluation of paints: density, viscosity, brushability, spraying properties, covering power, opacity, drying time, volatile content, flash point, optical and mechanical properties of dry films.

7.4 Varnishes and lacquers: composition and uses, oleoresinous varnishes, defects in varnish films.

7.5 Control of volatile organic emulsions in paint industry.

Module 8: Miscellaneous Oil and Fat Products (9 Hrs)

8.1 Sulphonated oils- sulphonation process, applications of sulphonated oils.

8.2 Linoleum, oiled fabrics, miscellaneous fat-based products: manufacture and utilization of nitrogen, phosphorous and sulfate containing products.

Module 9: Instrumental methods of Analysis (9 Hrs)

9.1 Applications of a) Refractometry, b) Dilatometry, c) Polarography, d) X-ray diffraction.

9.2: Surface Study Techniques - Instrumentation and Applications of Microscopic methods: SEM, TEM, STM, AFM.

References

[1] D. Swern, Bailey's Industrial Oil and Fat Products, Vol. I and II, 4th Edn., John Wiley, 1982.

[2] T.H. Applewhite, Bailey's Industrial Oil and Fat Products, Vol. III, 4th Edn., John Wiley, 1985.

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PG4APL E03 ESSENTIAL OILS AND AROMATICS

Credit: 4 **Contact lecture hours: 90**

Module 1: Essential oils (18 Hrs)

1.1 Production and isolation of essential oils. General methods for the production of essential oils- methods of isolation, theories of distillation, hydro distillation (water distillation, water and steam and steam distillation), solvent extraction, enfleurage, maceration, expression, supercritical fluid extraction, advantages and applications.

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

Module 2: Terpenoids (9 Hrs)

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

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

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

Hydrocarbons: Ocimene, p-Cymene, Limonene, Carene, Pinene, Camphene, Fenchene, Bisabolene, Zingiberene, Caryophyllene.

Alcohols: Linalool, Geraniol, Citronellol, Terpineol, Menthol, Borneol, Isoborneol, Farnesol, Fenchyl alcohol, Sandalols, Leaf alcohol.

Aldehydes: Citral, Citronellal, hydroxyl citronellal.

Ketones: Methyl Heptenone, Menthone, Piperitone, Pulegone, Carvone, Fenchone, Camphor, Ionones, Irones.

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

Module4: Study of essential oil constituents- II (18 Hrs)

Natural source, production, structure, properties and uses of aromatics and essential oil constituents such as: Alcohols: Benzyl alcohol, Phenyl ethyl alcohol, Cinnamyl alcohol, leaf alcohol

Aldehyde: Benzaldehyde, Phenyl acetaldehyde, Cinnamic aldehyde, Salicylaldehydes, Anisaldehyde, Vanillin, Piperonal.

Phenols: Thymol, Carvacrol, Eugenol, Isoeugenol, Methyl eugenol.

Acids and Esters: Cinnamic acid, Salicylic acid, Benzyl acetate, Benzyl benzoate, Cinnamyl acetate, Geranyl acetate, Linalyl acetate, Menthyl acetate, Amyl acetate.

Miscellaneous Compounds- Coumarin, Cineoles, Anethole, Ascaridole, Indole, Muscone, Civetone, Exalton, Artificial Musk.

Module 5: Spices and spice oils (9 Hrs)

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

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

Module 6: Flavour (9 Hrs)

6.1 Concept of flavour, Classification of flavours – Natural, Nature identical and synthetic. Alliaceous flavours- onion, garlic. Bittering agents- flavour of coffee, green tea, black tea and cocoa. Evolution of flavours during processing – enzymatic development, effect of roasting. Difference between perfume and flavour.

6.2 Sensory analysis- descriptive and discriminant sensory analysis, total component analysis, basics and methods, recent developments. Head space analysis, static and dynamic methods, basic principles, method and developments. Solid phase micro extraction of aroma components. E nose technology. Tristimulus colorimetry- basics and application to foods.

Module 7: Chemistry of Perfumes. **(9 Hrs)**

7.1 Odour, Odorants, Olfaction, Classification of odour. General physiology of Olfaction. Perfume raw materials- terpeneless and sesqueterpenless oils, concrete oils, absolute oils, isolates from essential oils, tincture, balsams and resins. Source and chemical nature of commercially important gums, balsams and resins. Perfume technology- blending and formulation of perfumes. Aerosol spray perfumes.

7.2 Application of herbs in cosmetics application, preservation; Advantages in perfumery: Notes of perfume, compatibility of perfume, fixation and stability of perfume; analysis of perfumes, Medicinal applications of perfumes. Synthesis of vanillin, ionones, methyl ionones, jasmone.

References

[1] F. Rosengarten, The Book of Spices, Jove, 1981.

[2] J.W. Parry, Hand Book of Spices, Chemical Publishing, 1969.

[3] J.S. Pruthi, Spices and Condiments Chemistry, Microbiology and Technology, Academic Press, 1980.

[4] E. Guenther, The Essential Oils, Vol I-VI, Van Nostrand, 1972.

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PG4APL E04 - POLYMER CHEMISTRY

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

Module 1: Introduction to Polymer Science (9 Hrs)

1.1 History of macromolecular science: monomers, functionality, degree of polymerization, classification of polymers based on origin, structure, backbone, branching, action of heat, ultimate form and use, tacticity and crystalline behaviour.

1.2 Primary bonds-molecular forces in polymers: dipole forces, induction forces, dispersion forces and H bond, dependence of physical properties on intermolecular forces. Polymer molecular weight-different averages, polydispersity index, molecular weight distribution curve, polymer fractionation. Methods for molecular weight determination: end group analysis, colligative property measurements, ultracentrifugation, vapour phase osmometry, viscometry, GPC, light scattering method. Monomers and structure of common polymers like PE, PP, PVC, PVAc, PVA, PMMA, PEMA, poly lactic acid, PET, PBT, PS, PTFE, PEI, nylon 6, nylon 66, nylon 612, Kevlar, PEEK, PES, PC, ABS, PAN, PEO, PPO, PEG, SAN, PCL, PLA, PHB, DGEBA, MF, UF, AF, PF, PU, NR, SBR, NBR, PB, butyl rubber, polychloroprene and thiokol rubber.

Module 2: Fundamentals of Polymerization (18 Hrs)

2.1 Addition polymerization, free radical addition polymerization, mechanism and kinetics of vinyl polymerization, kinetics of free radical addition polymerization, effect of temperature, pressure, enthalpies, entropies, free energies and activation energies on polymerization.

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

2.3 Mechanism of coordination polymerization, Ziegler-Natta polymerization, ring opening polymerization, mechanism of polymerization of cyclic amides.

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

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

2.6 Controlled polymerization methods, nitroxide mediated polymerization, Ring Opening polymerization (ROP), Atom Transfer Radical Polymerization (ATRP), Reversible Addition Fragmentation Termination (RAFT).

Module 3: Properties of Polymers (18 Hrs)

3.1 Structure property relationship in polymers, transitions in polymers, first order and second order transitions in polymers, relationship between Tg and Tm, molecular motion and transitions, Boyer-Beamem rule, factors affecting glass transition temperature.

3.2 Rheological properties of polymers, Newtonian fluids, non-Newtonian fluids, pseudoplastic, thixotropy, St. Venant body, dialatant, complex rheological fluids, rheopectic fluids, time dependent fluids, time independent fluids, power law, Weissenberg effect, laminar flow, turbulent flow, die swell, shark skin, viscous flow.

3.3 Viscoelastic properties of polymers, viscoelasticity, Hooke's law, Newton's equation, viscoelastic models-time temperature equivalence, WLF equation, Boltzmann superposition principle, linear stress - strain relations for other types of deformation-creep, stress relaxation. Temperature dependence of viscosity. Transport in polymers - diffusion, liquid and gas transport, Fick's law, theories of diffusion.

Module 4: Stereochemistry and Conformation of Polymers (9 Hrs)

4.1 Stereoregular polymers, constitutional isomerism, positional isomerism and branching, optical isomerism, geometric isomerism, substitutional isomerism, configuration of polymer chains, infrared, Raman and NMR characterization, polymer conformation, chain end to end distance, random walks and random flights, self-avoiding walks.

Module 5: Morphology and Order in Crystalline Polymers (9 Hrs)

5.1 Polymer morphology, common polymer morphologies, structural requirements for crystallinity, degree of crystallinity, crystallisability-mechanism of crystallization, polymer single crystals, lamellar structure of polymers, fringed micelle concept, folded chain model, adjacent re-entry model, switchboard model.

5.2 Structure of polymers crystallised from melt, spherulitic morphology, mechanism of spherulite formation, theories of crystallisation kinetics, Avrami equation, Hoffman's nucleation theory, the entropic barrier theory, strain induced morphology, cold drawing, morphology changes during orientation, application of XRD, SEM and DSC in determining the crystallinity of polymers.

Module 6: Advances in Polymers (9 Hrs)

6.1 Specialty polymers, conducting polymers, high temperature polymers, flame resistant polymers, biopolymers and biomaterials, polymers in medicine, polymers for dental applications

6.2 Carbon fibres. Synthesis, characterization and applications of carbon nanofibres.

Module 7: Dendrimers and Dendritic Polymers (18 Hrs)

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

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

7.3 Characterisation of dendrimers: GPC, osmosis, TG, DSC, magnetic resonance spectroscopy (proton and carbon-13 NMR), mass spectral studies (MALDI and TOF).

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

References

[1] V.R. Gowariker, N.V. Viswanathan, J. Sreedhar, Polymer Science, New Age International, 2003.

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PG4APL E05 ANALYTICAL CHEMISTRY

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

Module 1: Instrumental Methods (36 Hrs)

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

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

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

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

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

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

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

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

Module 2: Sampling (18 Hrs)

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

2.2 Decomposition and dissolution, source of error, reagents for decomposition and dissolution like HCl, H_2SO_4, HNO_3, $HClO_4$, HF, microwave decompositions, combustion methods, use of fluxes like Na_2CO_3, Na_2O_2, KNO_3, NaOH, $K_2S_2O_7$, B_2O_3 and lithium metaborate. Elimination of interference from samples-separation by precipitation, electrolytic precipitation, extraction and ion exchange. Distribution ratio and completeness of multiple extractions. Types of extraction procedures.

Module 3: Applied Analysis (9 Hrs)

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

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

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

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

Module 4: Capillary Electrophoresis and Capillary Electro Chromatography (9 Hrs)

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

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

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

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

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

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

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

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

References

[1] J.M. Mermet, M. Otto, R. Kellner, Analytical Chemistry, Wiley-VCH, 2004.

[2] D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College Pub., 2007.

[3] R.D. Brownn, Introduction to Instrumental Analysis, McGraw-Hill, 1958.

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[8] E.D. Howe, Fundamentals of Water.

SEMESTERS 3 & 4

PG4APL P04- INDUSTRIAL OIL AND FAT PRODUCTS PRACTICAL

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

I. Analysis of Vanaspati:

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

II. Soap analysis:

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

III. Glycerine analysis:

Analysis of glycerine for specifications-glycerine content, ash, total residue, acidity/alkalinity.

IV. Preparation of different types of soaps:

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

b) Preparation detergent powder, shampoo, vanishing cream.

V. Viva-voce

References

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

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

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

PG4APL P05 - ESSENTIAL OILS AND AROMATICS PRACTICAL

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

I. Preparation of essential oils

1. steam distillation
2. solvent extraction
3. enfleurage.

II. Assay of essential oils and perfumery materials

1. Determination of specific gravity, refractive index, optical rotation, boiling point and boiling range. Fractionation and solubility.
2. Estimation of essential oil constituents in the following.

   01. Citral in lemongrass oil; 02. Cinnamaldehyde in cinnamon oil; 03. Methyl salicylate in wintergreen oil; 04. Cineole in eucalyptus oil; 05. Eugenol in clove oil; 06. Estimation of vanillin; 07. Estimation of aldehydes in lemon grass oil.

III. Detection and estimation of common adulterants

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

IV. Preparation of some typical isolates from essential oils

01. Citral from lemongrass oil, 02. Cineol from eucalyptus oil, 03. Cinnamaldehyde from cinnamon oil, 04. Eugenol from clove oil.

V. Synthesis and spectral analysis

Synthesis of aromatics and perfumery compounds by conventional method/ Green method and prediction of FTIR, ^{1}H and ^{13}C NMR spectra of the substrates, intermediates and products at each stage of the products synthesized by the above methods.

Nerolin, β- ionone, Methyl cinnamate, Benzyl acetate, Amyl benzoate, Coumarin, Amyl isovalerate, Amyl salicylate, Chalcone.

VI. Viva-voce

References

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

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

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[11] J. B. Cohen, Practical Organic Chemistry, McGraw Hill.

PG4APL P06- FIXED OILS AND FATS PRACTICAL

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

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

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

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

II. Special test for oils

Stoke's test and Bailey's test for Castor oil, test for detection of Peanut oil, color test for cotton seed oil and sesame oil.

III. Detection of common adulterants in oils and fats

Detection of Vanaspati in butter and ghee.

IV. Colorimetric estimation of cholesterol in fats

V. Preparation based on oils and fats

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

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

VI. Viva-voce

References

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

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

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