Maharaja's College Ernakulam

A GOVERNMENT AUTONOMOUS COLLEGE

Re-Accredited by NAAC with 'A Grade'
Affiliated to Mahatma Gandhi University
Centre of Excellence under Govt. of Kerala
Identified by UGC as College with Potential for Excellence

POST GRADUATE & RESEARCH DEPARTMENT OF CHEMISTRY

Post Graduate Curriculum and Syllabus

(All Branches)

For 2019 Admission Onwards

M.Sc. APPLIED CHEMISTRY

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 organized 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, Dr. Lissamma Koshy, Associate Professor (Retd.), Maharaja's College, Ernakulam and Dr. Anitha I, Principal, KKTM College, Pullut 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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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)

a) Evaluation of Assignment

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

b) 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

$$CGPA = \sum(TCP \times TC) \div \sum TC$$

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. 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	3	20	80	100
		Total	**25**	**450**	**24**			
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		100	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)

4.1. 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 – Structure and bonding of 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.

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

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PG1 APL 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), 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, cyanohydrin 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 Stereoisomerism: Definition based on symmetry and energy criteria. Projection formulae. Configurational isomerism. Geometrical isomerism- nomenclature, methods of determination of geometrical isomers based on physical properties, NMR spectroscopy and chemical methods. Optical isomerism, nomenclature.

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

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 Chiral drugs.

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. Bridged bicyclic systems- norbornane, camphor, bicyclo[2.2.2]octane.

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.

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PG1 APL 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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PG1 APL 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 andvolume. 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.

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

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SEMESTER 2

PG2 APL C05 INORGANIC CHEMISTRY- II

(BIOINORGANIC & ORGANOMETALLIC CHEMISTRY)

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

Module 1: Bioinorganic Compounds (18 Hrs)

1.1 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.

1.2 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.

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

Module 2: Inorganic Chains (9 Hrs)

2.1 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.

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: Stereochemistry of Coordination Compounds (9 Hrs)

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

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

Module 5: Reactions of Organometallic Compounds (9 Hrs)

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

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

5.3 Rearrangement reactions, redistribution reactions, fluxional isomerism.

Module 6: Catalysis of Organometallic Compounds (9 Hrs)

6.1 Alkene hydrogenation, Tolman catalytic loop, Synthesis gas, Hydroformylation, Monsanto Acetic acid process, Wacker process, Zeigler Natta catalysis.

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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PG2 APL 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, 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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[2] F.A. Carey, R.A. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th Edn., Springer Science & Business Media, 2007.

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PG2 APL 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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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

PG2 APL 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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SEMESTERS 1 AND 2

PG2 APL 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.

PG2 APL 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.

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

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

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PG2 APL P03 PHYSICAL CHEMISTRY PRACTICAL - 1

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

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

Part A

I. Adsorption

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

II. Phase diagrams

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

III. Distribution law

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

IV. Surface tension

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

3. Determination of the composition of two liquids by surface tension measurements.

Part B

Computational Chemistry Experiments

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

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

References

[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.

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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

[1] M.B. Smith, Organic Synthesis, 3rd Edition, Wave functions Inc., 2011.

[2] F.A. Carey, R.I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edn., Springer, 2009.

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[17] R.C. Larock, Comprehensive Organic Transformations, VCH, 1989.

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[19] J. Zhu, Q. Wang, M. Wang (Eds), Multicomponent Reactions in Organic Synthesis, Wiley VCH, 2015

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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

[2] F.W. Sears, G.L. Salinger, Thermodynamics, Kinetic Theory and Statistical Thermodynamics, Addison Wesley, 1975.

[3] J. Kestin, J.R. Dorfman, A Course in Statistical Thermodynamics, Academic Press, 1971.

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[5] K. J. Laidler, Chemical Kinetics, 3rd Edn., Harper & Row, 1987.

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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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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, ^{19}F and ^{31}P NMR.

3.4 2D NMR and COSY, HOMOCOSY and HETEROCOSY

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

3.6 Problems on spectral interpretation with examples.

Module 4: Mass Spectrometry (9 Hrs)

4.1 Molecular ion: ion production methods (EI). Soft ionization methods: SIMS, FAB, CA, MALDI, 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

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

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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.

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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.

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.

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.

[2] T.H. Aplewhite, Bailey's Industrial Oil and Fat Products, Vol. III, 4th Edn., John Wiley-Interscience,1985.

[3] F.D. Gunstone, An introduction to Chemistry and Biochemistry of Fatty acids and their Glycerides, Chapman and Hall, 1968.

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[6] P. Tooley, Chemistry in Industry-Fats, Oils and Waxes, John Murray, 1971.

[7] W.W. Christie, Lipid Analysis, 3rd Edn., Oily Press, 2003.

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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.

[3] E.S. Pattison, Fatty acids and their Industrial Applications, Marcel Dekker, 1968.

[4] A.J.C. Andersen, Refining for Oils and Fats for Edible Purposes, Pergamon Press, 1962.

[5] C.R. Martens, Emulsion and Water soluble Paints and Coatings, Reinhold, 1964.

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[10] H.H. Willard, L.L. Merritt, J.A. Dean, Instrumental Methods of Analysis, 5th Edn.

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[12] Niir Board, Modern technology of oils, fats and its derivatives, Asia pacific business.

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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[11] I.L. Finar, Organic Chemistry, Vol. II, 7th Edn, Pearson Education, 2004.

[12] H. Panda, Perfumes and Flavours Technology Hand Book,2010.

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.

[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.

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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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[6] J.H. Kennedy, Analytical Chemistry: Principles, Saunders College Pub., 1990.

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SEMESTERS 3 AND 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.

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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.

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

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

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

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

[7] V.K. Ahluwalia, Green Chemistry: Environmentally Benign Reactions, Ane Books, 2009.

[8] Monograph on Green Chemistry Laboratory Experiments, Green Chemistry Task Force Committee, DST, 2009.

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

[10] F. G. Mann and B.C. Saunders, Practical Organic Chemistry, Pearson.

[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.

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

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

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

M.Sc. Degree Applied Chemistry Programme

Aim and Objective of the Syllabi

Aim

Chemistry is a central subject of science. It is also closely related to daily life. The Master's program not only offers the option of focusing on a specialist area but students will also acquire the necessary skills for this and they will learn to think independently and act responsibly.Graduates will become familiar with the terminologies and special aspects of chemistry, its strengths and limitations and will be able to apply their knowledge to new issues and situations, even in an interdisciplinary context. They will gain knowledge and practical skills relating to the current state of research in selected fields. They will be able to analyze chemical issues and assess them critically, to develop independent solution strategies and to estimate their impacts in a wider context.The broad spectrum of the academic program will ensure that students acquire the skills necessary for demanding fields of activity in industry, economy and administration

Objective

The Master's course in chemistry is designed with an objective to teach post graduates with the skills to critically assess and deal with issues requiring the utilization of chemical principles from each sub-disciplines such as organic, inorganic, physical, analytical and biochemistry. It is the objective of the chemistry program to teach students the necessary knowledge in a way that enables them to familiarize themselves quickly with new developments, to be introduced to new areas and to make independent contributions to further developments of research and technology in their specialized area once they have finished their program.

PG1APL C01 Inorganic Chemistry - I

Aim and Objectives

This is a chemistry module designed for chemistry majors and featuresthe principles of coordination chemistry, boron compounds and that of nuclear chemistry.In depth discussion about coordination compounds focusing primarily on their structure and various aspects of bonding will be done. The course covers synthesis, structure and bonding of organometallic compounds. Kinetics of reactions of metal complexes and their mechanism will also be illustrated. The learners should be able to apply these topics in various fields.

PG1APL C02 Organic Chemistry - I

Aim and Objectives

The module deals primarily with the basic principles to understand the structure and reactivity oforganic molecules. Emphasis is on substitution and elimination reactions of aliphatic and aromatic compounds. Learners will get the essential ideas on how simple molecules can beconstructed. Bonding in conjugated systems, reactions mechanism, organic transformations and stereochemistry will likewise be discussed.

PG1APL C03 Theoretical Chemistry - I

Aim and Objectives

This module looks at quantum chemistry and group theory. A more profound comprehensionof quantum chemistry beginning from its postulates and basic systems such as particle-in-a-box to hydrogen like atoms is explored. The second part of the module looks at molecular symmetry and applications in molecular orbitals analysis and vibrational spectroscopy, electronic transitions of carbonyl chromophore and origin of selection rule of electronic transition. Learners will be able to apply these ideas to individual atoms and molecular systems.

PG1APL C04 Physical Chemistry - I

Aim and Objectives

Physical chemistry is the study of phenomena in chemical systems in terms of physical conceptsand laws. In this module,different branches of thermodynamics will be explored. In *ClassicalThermodynamics*

kinetic theory of gases, and the energetics of chemical reactions will be explored. Thermodynamics of natural processes and energy transformations in living organisms will be discussed in *Irreversible thermodynamics*. *Statistical Thermodynamics* looks at the relationship between molecular and bulk properties of matter, including examples such as the use of partitionfunctions in equilibrium, transition states and heat capacity of chemical systems. Learners will be familiarized with the behavior of matter in bulk.

PG2APL C05 Inorganic Chemistry - II
Aims and Objectives
This module coversthree parts: non-aqueous solvents, bioinorganic chemistry and organometallic chemistry. Part 1 deals with acid-base concept and reactions in non-aqueous solvents.Part 2 describes basic principles and concepts of bioinorganic chemistryincluding the mechanisms of reactions catalyzed by metalloproteins, and kinetics of electron transfer in proteins. Part 3 focusses on thespectral and magnetic properties of transition metal complexes. A comprehensive discussion on inorganic cages and metal clusters follows. The learners will understand the different modes of reactions oforganometallic compounds and their applications can be explored.

PG2APL C06 Organic Chemistry - II
Aim and Objectives
This module covers the study of a selected series of organic reactions involving reactiveintermediates and/or molecular rearrangements. Emphasis is placed on an understanding oftheir reaction mechanisms. These will include reactions involving carbocations, carbanions, carbenes, carbenoids, nitrenes and arynes as intermediates. Reactions initiated by radicals will be covered.Comprehensive discussions on organic photochemistry including the rules and stereochemical consequences in pericyclic reactions willbe given. The learners should be able to apply these ideas in the field of organic synthesis.

PG2APL C07 Theoretical Chemistry - II
Aim and Objectives
The objective of this model is to familiarize the learner with the approximation methods of quantum mechanics and its applications to the various theories of chemical bonding. Molecular structure evaluation using group theory will enable the learners to apply it in the field of spectroscopy. To apply the concept of molecular modelling to isolated molecular systems.

PG2APL C08 Physical Chemistry - II
Aim and Objectives
In this module, the basic idea of how light interacts with matter, in particular atoms and moleculeswill be conferred. Microwave, infrared, Raman, electronic and nuclearmagnetic resonance spectroscopic techniques will be discussed. Students will be able to apply these principles in the area of molecular spectroscopy.

PG1APL P01 Inorganic Chemistry Practical- I
Aim and Objectives
This is a module intended for chemistry majors. It deals with qualitative and quantitative inorganic analysis along with preparation and characterization of inorganic complexes. The learners will have the option to apply these ideas in various fields pertaining to inorganic chemistry.

PG2APL P02 Organic Chemistry Practical- I
Aim and Objectives
In this module,students will learn to apply various techniques to separate a mixture into its individual components and identify each component. Guided under the general principles of analytical and physical chemistry, these techniques include solvent extraction, TLC and column chromatography. Students will also acquire the skill to use the computational tools to draw the reaction schemes and mechanisms of various organic reactions.

PG2APL P03 Physical Chemistry Practical- I
Aim and Objectives
In this module,students will learn about the practical applications of variousprinciples of physical chemistry like phase rule, adsorption, and surface tension.Learners will be able to use computational software to predict the geometry of a molecule, calculate its energy levels, assess the HOMO and LUMO energy, and predict its spectral behavior.

PG3APLC09 Organic Chemistry-III (Organic Synthesis)
Aim:

Course Outcomes:

- To identify the basic principles, terminology and important strategies of retro synthesis
- To make awareness about the reagents and basic organic reactions
- To study the influence of light and thermal energy for the formation of cyclic systems
- To aware of basic ideas and applications of supramolecular chemistry
- To understand the structure determination and synthesis of natural products

Course Objectives:

- To identify the basic principles, terminology and important strategies of retro synthesis
- To make awareness about the reagents and basic organic reactions
- To understand the chirality, chiral catalyst and asymmetric synthesis
- To study the influence of light and thermal energy for the formation of cyclic systems
- To aware of basic ideas and applications of supramolecular chemistry
- To understand the structure determination and synthesis of natural products

PG3 APL C10 Physical chemistry- III (Selected topics in Physical Chemistry)
Objectives:

- To give an in-depth account of different theories of reaction rates, kinetics of fast reactions and reaction in solution.
- To study the different types of quantum statistics and its comparison, Laws related to heat capacity of solids, phase transition and thermionic emission.
- To study the chemistry of surfaces and various techniques employed for the characterization of different types of surface phenomena and the importance of adsorption process and catalytic activity at the solid surfaces
- To impart knowledge about acid-base, enzyme and surface catalysis.
- To impart knowledge about enzyme inhibition, protein folding and molecular motors.
- To recognize the general properties of colloids and macromolecules
- To acquire knowledge of photochemistry and photophysical principles, their applications

Outcome:

- The student will acquire knowledge about different theories on reaction rate, can analyse the mechanistic path and the experimental conditions of different types of reactions.
- Will able to understand the different techniques for analysing fast reactions.
- Will able to classify the particles according to different statistics and to do problems based on the arrangement of particles in different energy states.
- To compare the different laws related to heat capacities.
- To generate idea about phase transitions and thermionic emissions.
- Will acquire knowledge about the acid base catalysis, enzyme catalysis and their principles.
- Will appreciate the applications of chemical principles of surface catalysis and colloidal chemistry in industrial synthesis.
- Able to classify colloids present in nature and apply its properties in daily life.
- Apply the principles of adsorption in daily life situations.
- The student will able to apply photochemistry and photophysical principles on environmental and biological processes and will explain photophysical energy conversion to generate electricity
- Gains numerical ability and analysing power to solve problems.

PG3APL C11 (Fatty Acids, Nano and Green Chemistry)

Course Objectives:

- To understand the classification, nomenclature of lipids
- To study the functions and applications of fatty acids
- Identify various fatty acids
- Analyse various methods of separations of fatty acids
- Describe the applications of TLC and FID and spectroscopic analysis of triglycerides
- To understand the properties and biochemistry of fatty acids
- To study the importance of Nanomaterials and Green Chemistry

PG3APL C12 Spectroscopic Methods in Chemistry

Course Objectives:

- To understand the basic ideas of different spectroscopic Techniques
- To identify the compounds by analyzing the UV, IR NMR and Mass spectrum
- To interpret the spectrum of organic compounds
- To develop the structure elucidation skill of organic compounds using different types of spectral data

PG4APL E01- Analysis of Fats, Oils and Waxes

Course Objectives

- To make an awareness of the different methods of extraction of oils and fats
- To understand the source and utilization of different types of oils and fats
- To understand the structure and synthesis of glycerides
- To study the physical and chemical properties fats and oils
- To develop the chemistry and functions of nonglyceride constituents of fats and oils
- To study the occurrence, classification, properties and composition of waxes and drying oils

PG4APL E02 Industrial Oil and Fat Products

Course objectives:

- To make an awareness of the processing of oils and fats

- To understand the hydrogenation oils
- To understand the esterification reactions of fats
- To study the applications of grease and lubricating oils
- To study the manufacture methods and analysis of soaps, shampoos and synthetic detergents
- To study the basic ideas of paint, varnish and lacquers
- To study the instrumental methods of analysis of oils and fats

PG4APL E03 Essential Oils and Aromatics
Course objectives:

- To make an awareness of the production and isolations of essentials oils and terpenoids
- To understand the constituents of essential oils
- To understand the source, production and chemical constituents of spices and spice oils
- To study the classification, preparation and applications of flavors
- To study the classification, preparation and applications of perfumes

PG4APL E04 - Polymer Chemistry
Course Objectives:

- To acquire the knowledge about different types of polymers
- To understand the different types of polymerization
- To study the physical and chemical properties of polymers
- To understand the morphology and order in crystalline polymers
- To study the advances in polymers
- To understand the basic ideas of denrimers and dentritic polymers

PG4APL P04- Industrial Oil and Fat Products Practical
Course Objectives:

- To develop skills in analysis of vanaspathi, soap and glycerin
- To understand the methods of preparation of different types of soap

PG4APL P05 - Essential Oils and Aromatics Practical
Course Objectives:

- To understand different techniques of extraction of essential oils
- To test the assay of essentials Oils and perfumery material
- To make awareness about detection and estimation of common adulterants in essential oils
- To study the synthesis of essential oils and distinguish by spectral analysis

PG4APL P06- Fixed Oils and Fats Practical
Course Objectives:

- To understand the experimental methods of the determination of physical chemical constants of oils and fats
- To make the skills of special tests of oils
- To find out the adulterants in oils and fats
- To prepare the common fatty acids involving chemical reactions