St Aloysius College (Autonomous)
Mangalore

Re-accredited by NAAC "A" Grade

Course structure and Syllabus

of

M.Sc. CHEMISTRY

CHOICE BASED CREDIT SYSTEM (CBCS)

(2021 –22 BATCH ONWARDS)

ಸಂತ ಅಲೋಶಿಯಸ್ ಕಾಲೇಜು
(ಸ್ವಾಯತ್ತ)
ಮಂಗಳೂರು– 575 003, ಕರ್ನಾಟಕ
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Re-accredited by NAAC with 'A' Grade with CGPA 3.62/4
Ranked 95 in College Category – 2021 under NIRF, Ministry of Education, Government of India
Recognised as Centre for Research Capacity Building under UGC-STRIDE Scheme
Recognized under DBT – BUILDER Scheme, Government of India
College with "STAR STATUS" Conferred by DBT, Government of India
Recognised by UGC as "College with Potential for Excellence"

Date: 12-08-2021

NOTIFICATION

Sub: Syllabus of **M.Sc. Chemistry** under Choice Based Credit System.

Ref: 1. Decision of the Academic Council meeting held on 19-06-2021vide Agenda No: 20 (1) (2021-22)
2. Office Notification dated 12-08-2021

Pursuant to the above, the Syllabus of **M.Sc. Chemistry** under Choice Based Credit System which was approved by the Academic Council at its meeting held on 19-06-2021 is hereby notified for implementation with effect from the academic year **2021-22.**

PRINCIPAL **REGISTRAR**

To:

1. The Chairman/Dean/HOD.
2. The Registrar Office
3. Library
4. PG Office

PREAMBLE:

St. Aloysius College established in 1880 as a minority institution is managed by the Jesuit Fathers of Mangalore Educational Society (MJES). The college was conferred autonomy from the academic year 2007-08. The Department of Chemistry, a pioneer in Chemistry education in the district, aims at building total personality of the student transforming young boys and girls into men and women for others, having compassion concern and commitment to the society. The M.Sc Course in analytical chemistry is an added commitment to the cause of higher education with an aim of serving the community. The course was started under the affiliation of Mangalore University and now is brought under Autonomy. Hence though the same syllabus has been retained with minor modifications, structural changes are incorporated to suit the credit system under autonomy.

OBJECTIVES:

- To provide knowledge and skills in the field of analytical chemistry
- To generate manpower trained in analytical chemistry to meet the need of industry and academia.
- To train students to pursue research in the field of chemistry.
- To impart training in laboratory skills.
- To develop the personality of an individual by giving them the necessary skills.
- To offer 100% placement assistance.

SCOPE OF THE COURSE:

M.Sc in General chemistry is a post graduate course with job opportunities in industry, teaching and research. The Research and Development section of every industry requires personnel who are trained in and handling various instruments. The course structure and curriculum is designed to enable the students to develop analytical and creative abilities which are very much needed by the industry and enable them to face national level competitive exams. The Course is definitely at par with M.Sc Organic Chemistry, M.Sc Analytical chemistry, M.Sc Medicinal Chemistry etc.

COURSE INTAKE:

The maximum number of students to be admitted to the course is 30 each year.

ELIGIBILITY

- Candidates would have studied any branch of Physical or biological science with chemistry as one of the major / optional subject in the under graduate level
- Not less than 45%(40% in case of SC/ST students) marks in the aggregate excluding languages in the under graduate level.
- The students should have studied physics and Mathematics at the higher secondary level.

SYLLABUS

- The course will be conducted in accordance to the semester system
- Each semester consists of 20 weeks inclusive of examinations.
- All examinations including practical/ project/viva will conclude by the end of the 20th week.
- A candidate should secure overall a minimum 40% marks in each paper, including both internal assessment and end semester examination.
- A minimum of 35 % in each paper of end semester examination
- 75% attendance is the minimum requirement for appearing for the semester examinations

EVALUATION SYSTEM

- The evaluation system of the course is based on two components. (i) Continuous evaluation (ii) End semester Examination.
- Continuous Evaluation: Based on this Internal assessment marks are allotted. It includes the following criterion-
- 50% marks for two internal assessment examination- Two examinations of 1 hour 30 minutes duration each carrying 50 marks in each semester are conducted. Total marks secured are reduced to 25.
- 3 marks are given for class participation.
- 7 marks are allotted for class seminar and 5 marks for quiz
- Ten marks for writing assignments and reviews.

- In the practicals of the first and second semester, one model examination is conducted for 40 marks and 10 marks for the viva. The marks are reduced to 25, continuous evaluation is done for 12 marks, 10 marks for class records and 3 marks for class participation. These marks are reduced to 15.

- In the practicals of the third and fourth semester, one model examination is conducted for 40 marks and 10 marks for viva. The marks are reduced to 25, continuous evaluation is done for 12 marks, 10 marks for class records and 3 marks for class participation. These marks are reduced to 30

END SEMESTER EXAMINATION

- Each end semester examination is conducted out of 70 marks. End semester examination question paper consists of questions to assess the conceptual, comprehensive and analytical abilities of the students.

- In all four semesters end semester practical exam is conducted in 50 marks

(40 marks for practical proper and 10 marks for the viva) and the marks are reduced to 35.

THEORY QUESTION PAPERS PATTERN

- The Syllabus of each paper shall be grouped into units of 14 teaching Hours.

- All hard core papers will have 4 units. Soft core and open elective papers will have 3 units.

- Question Papers in all the four semesters shall consist of Parts A and B.

- For hard core papers - Part A shall contain eight (8) very short answer objective type questions carrying 2 marks each drawn from all the four units of the syllabus (2 questions per unit). Five (5) questions are to be answered.

- Part B shall contain eight (8) brief and/or long answer questions carrying 12 marks each drawn from all the four units of the syllabus (2 questions per unit).

- For soft core and open electives Part A shall contain 9 very short answer objective type questions carrying 2 marks each drawn from all the three units of the syllabus (3 questions per unit). Seven (7) questions are to be answered.

- Part B shall contain six (6) brief and/or long answer questions carrying 14 marks each drawn from all the three units of the syllabus (2 questions per unit).
- There may be a maximum of four sub-divisions per question, carrying 3 or more marks per sub-division. Five (5) out of eight (8) questions for hard core while 4 out of 6 questions for soft core and Open electives are to be answered choosing at least one question from each unit.

PROJECT WORK

- The project work shall be carried out in the last semester for 75 Hours.
- Can be carried out either in the institution or in an Approved Industry or in both.
- To be carried out under the supervision of a teacher and submit a project report.
- Experts from the industries may also be involved in the project work as co-guides and in the evaluation of project reports.

Evaluation

Project will be evaluated for hundred marks which includes presentation of the project.

Structure, Credits and Scheme of Examination of the Postgraduate Courses under Choice Based Credit System

M.Sc. Chemistry 2021

I Semester = 3 Hard core and 1+5 soft core paper

Code	Papers	Hours/ Week	Duration of Exam	Marks		Total	Credits
				IA	End Sem		
PH 581.1	Inorganic Chemistry	4	3	30	70	100	4
PH 582.1	Organic Chemistry	4	3	30	70	100	4
PH 583.1	Physical Chemistry	4	3	30	70	100	4
PS 584.1	Principles of Analytical Chemistry & Separation Techniques or	3	3	30	70	100	3
PS 585.1	Bioorganic Chemistry						
PS 586.1	Research Methodology	3	3	30	70	100	3
PS 587.1P	Inorganic Chemistry - Practicals – I	4	4	15	35	50	2
PS 588.1P	Organic Chemistry Practicals – I	4	4	15	35	50	2
PS 589.1P	Physical Chemistry Practicals – I	4	4	15	35	50	2
						650	**24**

II Semester = 3 Hard core and 1+4 soft core paper and open elective 1 paper

PH 581.2	Advanced Inorganic Chemistry	4	3	30	70	100	4
PH 582.2	Advanced Organic Chemistry	4	3	30	70	100	4
PH 583.2	Advanced Physical Chemistry	4	3	30	70	100	4
PS 584.2	Molecular Symmetry and Molecular Spectroscopy **Or**	3	3	30	70	100	3
PS 585.2	Chemistry of Biomolecules						
PS 586.2P	Inorganic Chemistry Practicals – II	4	4	15	35	50	2
PS 587.2P	Organic Chemistry Practicals – II	4	4	15	35	50	2
PS 588.2P	Physical Chemistry Practicals – II	4	4	15	35	50	2
PO 589.2	**Spectral Methods Of Analysis**	3	3	30	70	100	3
						650	**24**

M.Sc. Chemistry

III Semester = 2 Hard core and 1+4 soft core paper open elective 1 paper

Code	Papers	Hours/ Week	Duration of Exam	Marks		Total	Credits
				IA	End Semester		
PH 581.3	Organometallic, Bioinorganic and Coordination Chemistry	4	3	30	70	100	4
PH 582.3	Electrochemistry and Thermo- Analytical Methods	4	3	30	70	100	4
PS 583.3	Molecular Spectroscopy or	3	3	30	70	100	3
PS 584.3	Medicinal Chemistry						
PS 585.3P	Computers for Chemists - Practicals	4	4	15	35	50	2
PS 586.3P	Inorganic Chemistry Practicals- III	4	4	15	35	50	2
PS 587.3P	Organic Chemistry Practicals- III	4	4	15	35	50	2
PS 588.3P	Physical Chemistry Practicals- III	4	4	15	35	50	2
PO 589.3	Bio-Inorganic Chemistry, Green Chemistry And Environmental Chemistry	3	3	30	70	100	3
						600	**22**

IV Semester = 2 Hard core and 1+4 soft core paper open elective 1 paper

PH 581.4	Organic Synthetic Methods	4	3	30	70	100	4
PH 582.4	Radiation and Photochemistry	4	3	30	70	100	4
PH 583.4	Chemistry of Polymers and Natural Products	4	3	30	70	100	4
PS 584.4P	Organic Chemistry Practicals - IV	4	4	15	35	50	2
PS 585.4P	Inorganic Chemistry Practicals - IV	4	4	15	35	50	2
PH 586.4	Project Work	6	6	30	70	100	3
PS 587.4	Solid state and Nano Chemistry Or	3	3	30	70	100	3
	OR						
PS 588.4	Optical Methods of Analysis						
	Total					**600**	**22**
	Grand Total						**92**

NOTE: The First, Second and Third Semesters of the course involve theory and practical, while the IV Semester involves theory, practical and project work. The project work shall be carried out in the fourth semester for 75 Hours. After the Second Semester of the course, the project work could be carried out either in the institution or in an Approved Industry or in both. This should be under the supervision of a teacher and the project report should be submitted. Experts from the industries may also be involved in the project work as co-guides and in the evaluation of project reports.

MAIN FEATURES OF THE COURSE:

M.Sc Analytical chemistry has the following features.

❖ The entire course will have a total of 2500 marks with 92 credits distributed in 4 semesters. Out of 92 credits, hard core has 50 credits (54.34%), Soft core has 36 credits (39.12%), Open elective has 6 credits (6.54%)

First semester	650 Marks	24 credits
Second semester	650 Marks	24 credits
Third semester	600 Marks	22 credits
Fourth semester	600 Marks	22 credits
	2500 Marks	92 credits

FIRST SEMESTER

PH 581.1: INORGANIC CHEMISTRY

Course Outcome:

Student will be able to:

- **Explain the chemistry of acids, bases, non-aqueous solvents and** the concepts of hard and soft acids and bases
- Describe the types of bonds and molecular shape of compounds with emphasis on VSEPR, VB and MO theory of complexes.
- **Discuss the properties of the non-transition elements like C, B and Si and the**ir **frameworks**
- Illustrate the properties and justify the anomalies of Nitrogen, Phosphorus, Sulphur and noble gas compounds.

UNIT I : **14 hours**

Electronic configuration of atoms, Auf Bau principle, Pauli's exclusion principle, Hunds rule, Slaters rule of the determination of screening constants. Trends in atomic & ionic radii, IP & EA along the period,

Hydrogen bond: types and detection. Intermolecular Forces: Ion-dipole, dipole dipole, ion-induced dipole, dipole-induced dipole interactions and London forces.

Ionic bond: Properties of ionic substances, coordination number of an ion, structures of crystal lattices- NaCl, CsCl, ZnS and Rutile. Lattice energy- Born Lande equation, Born-Haber cycle, Uses of Born-Haber type of calculations. Ionic radii, methods of determining ionic radii, factors affecting ionic radii, radius ratio rule, covalent character in ionic bonds.

Covalent bond: valence bond theory, formal charge, resonance, hybridization, Bent's rules and energetics of hybridization, Deduction of molecular shapes – VSEPR theory, MO theory, application to homo (F_2 and N_2) and hetero diatomic (CO) and triatomic molecules (BeH_2 and nitrite ion).

UNIT II : **14 hours**

Review of acid- base concepts: Arrhenius theory, Bronsted-Lowry theory, Lewis theory, General properties of solvents. Classification of solvents.Factors justifying the need of Non Aqueous solution Chemistry and failure of water as a Solvent.

Acids and Bases: Measures of acid-base strength, Factors affecting strengths of hydracids, oxoacids and Lewis acids and bases, Drago -Wayland equation for Lewis acid- base interactions. hard& soft acid-bases, Lux-Flood, Usanovich & solvent system definition of acids and bases, solvent leveling effect, HSAB concepts, Symbiosis. Super acids - Hammet acidity function, Superacids based on arsenic and antimony

Non-aqueous solvents : Molten salts as solvents, ionic liquids, liquid NH_3 and liquid SO_2 as solvents, reactions in liq NH_3&liq SO_2, anhydrous H_2SO_4, glacial acetic acid as solvents,anhydrous HF, liquid sulphur dioxide

UNIT III : **14 hours**

Diagonal relationship between Boron & Silicon. Similarities in properties of Boron and Silicon.

Chemistry of higher boranes: Classification, types of bonds in higher boranes- the styx number, structures and M.O. description of bonding, framework electron counting, Wade's rules, chemistry of B_5H_9, $B_{10}H_{14}$ and $B_nH_n^{2-}$.

Carboranes : Classification, Wade's rules, nomenclature, structures of CB_5H_9, $C_2B_4H_8$, $C_3B_3H_7$ and $C_4B_2H_6$.

Borazines : Preparation, properties, structure. Difference in chemical properties between borazine and benzene, borazine derivatives (N & B substituted). Preparation of boron nitride.

Silicates : Classification, structure – Pyroxenes & amphiboles, Silicones, & zeolites.

UNIT IV : **14 hours**

Allotropes of nitrogen and sulphur, electronic configuration of N, P, S . Properties of inert gases and their oxidation states.

Hydrides, oxides and oxyacids of nitrogen, phosphorous, sulphur& halogens.

Phosphazenes- Classification, Cyclophosphazenes-$(NPCl_2)_3$ and $(NPCl_2)^{4-}$ preparation and structure, Linear polyphosphazenes- preparation and applications, phosphazene polymers. Sulphur-nitrogen compounds- Preparation and structures of S_4N_4 and S_2N_2 , $(SN)_x$

Condensed phosphates – linear polyphosphates, long chain polyphosphates and metaphosphates

Inter halogens, pseudohalogens, polyhalide ions, oxyhalogen species.

Noble gas compounds : Xenon oxides and fluorides. Preparation, properties and structures.

REFERENCES :

1. Inorganic Chemistry – Principles of Structure and Reactivity, J.E. Huheey, E.A. Keiter and R.L. Keiter, 4thEdn, Pearson Education Asia Pvt. Ltd., 2000.
2. Inorganic Chemistry, D.F. Shriver, P.W. Atkins and C.H. Langford, 2ndEdn, Oxford Univ. Press, 1994.
3. Concise Inorganic Chemistry, J.D.Lee, 5thEdn, Blackwell Science, 2000.
4. Basic Inorganic Chemistry, F.A. Cotton, G. Wilkinson and P. L. Gaus, 3rdEdn, John-Wiley and Sons, 1995.
5. Concepts and Models of Inorganic Chemistry, B. E. Douglas, D. McDaniel and A Alexander, Wiley, 2001
6. Chemistry of Elements, N.N. Greenwood and A.E. Earnshaw, Butterworth Heinemann, 1997.
7. Fundamentals of Inorganic Chemistry, Jack Barrett and Mounir A. Malati, Harwood, 1998.
8. Inorganic Chemistry-A Unified Approach, W. W. Porterfield, Elsevier, 2005.
9. Principles of Inorganic chemistry, Puri, Sharma and Kalia, 33rdEdn, Vishal Publishing House, 2016.
10. Selected Topics in Inorganic Chemistry, Madan and Tuli, 17th Edn, S Chand, 2010.
11. Inorganic Chemistry, Manku, 1stEdn, Tata- McGraw Hill, 2008.
12. Inorganic Chemistry, Meissler and Tarr, 5thEdn, Pearson, 2013.

PH 582.1 : ORGANIC CHEMISTRY

Course Outcome:

Student will be able to:

- Explain the basic concepts of organic chemistry and the forces of attraction between different molecules.
- Explain the reaction intermediates and mechanisms.
- Demonstrate the importance of conformation and stereochemistry in understanding the reactivity and stability of organic molecules
- Detail the synthesis and stereochemistry of carbohydrates

UNIT I **14 Hours**

Types of bonding, reactions (specify types), Bonds weaker than covalent: Hydrogen bonds types and applications, intermolecular forces; ion-dipole, dipole-dipole ion induced dipole, dipole-induced dipole interactions and London forces.

Nature of Bonding in Organic Molecules: Localized and delocalized bonding, Conjugation, cross conjugation, resonance, hyper-conjugation and tautomerism and inductive effects. Aromaticity in benzenoid and non-benzenoid molecules, Huckel rule, alternant and non-alternant hydrocarbons, Homo-aromatic and anti-aromatic systems. Annulenes and hetero-annulenes. Physical methods to study aromaticity-UV, IR & ^{1}H NMR. Addition compounds, Crown ether complexes and Cryptands inclusion compounds, cyclodextrins, Catenanes, rotaxanes and bonding in Fullerences

Acids and Bases : organic acids and bases, pKa and pH, effect of solvent on acid and base strength, effect of structure of organic compound on acid and base strength, relative strengths of acids and bases based on inductive, mesomeric and steric effects.

UNIT II **14 Hours**

Homolytic and heterolytic fission, carbanions and carbocations free radicals, relative stability.

Reaction Intermediates: Generation, structure, stability, reactivity and detection of classical and non-classical, carbenes, nitrenes and arynes(with at least two reactions for each type of intermediates). Structure and stability of Ylides and enamines.

Methods of Determining Reaction Mechanism: Identification of products, detection of intermediates, isotopic labeling, stereochemical evidences, cross-over experiments, kinetic evidences and kinetic isotopic effects.

UNIT III: **14 Hours**

Stereochemistry *Elements of symmetry, Chiral centres, chirality,Chiral molecules, Optical isomerism of lactic acid and tartaric acids.*

Optical Isomerism: Conformation and configuration of molecules, projection formulae, Ball & Stick and Barton Models, Fischer, Saw-horse, Newmann and Flying wedge representations. Absolute configuration (D,L) and (R,S) systems. Molecules with more than one chiral centre, threo and erythro isomers, methods of resolution, stereo specific and stereo selective synthesis, asymmetric synthesis, Cram's and Prelog's rules. Optical activity in the absence of chiral

carbon-biphenyls, allenes and spiranes. Stereochemistry of compounds containing nitrogen, sulphur and phosphorus. Conformational analysis of cycloalkanes and decalins. Effect of conformation on reactivity.

Geometrical Isomerism: Cis-trans isomerism resulting from double bonds, monocyclic compounds and fused ring systems. E Z-notations, determination of configuration of geometrical isomers, syn and anti-isomers

UNIT IV: **14 Hours**

Carbohydrates: Structural elucidation of fructose, Configuration and conformation of monosaccharide, Chemistry of important derivatives of monosaccharide-ethers, esters, acetals, ketals, deoxysugars, amino sugars. Structures of cellulose, chitin, starch, glycogen, heparin and chondritin.

Organic Name Reactions: Reactions, Mechanisms and synthetic uses of the following: Stobbe condensation, Darzen condensation, Gattermann-Koch reaction, Cannizzaro reaction,Duff reaction Chichibabin reaction, Benzoin condensation, Claisen-Schmidt condensation, Claisen reaction, Simon-Smith reaction, Stork Enamine reactions, Sharpless asymmetric epoxidation, Hofmann-Loffler-Freytag reaction, Woodward and Prevost Hydroxylation, Bucherer reaction, Ullmann reaction. Wittig reaction-Mitsunobu reaction, Stephen reaction.

REFERENCES:

1. Organic Chemistry- Claydon and Greaves, Oxford University Press, 2ndEdn, 2014

2. Advanced Organic Chemistry, Jagdamba Singh and LDS Yadav

3. Organic Chemistry, P.Y.Bruice, Pearson Education Pvt. Ltd.,New Delhi, 2002

4. Stereochemistry, Conformation and Mechanism, P.S.Kalsi, 6thEdn, Wiley Eastern, New Delhi, 2010

5. Stereochemistry of Carbon Compounds, E.L.Eliel, Tata McGraw Hill, New Delhi, 1994.

6. Organic Reaction Mechanisms, Fourth Edition,VK Ahluwalia and Rakesh kumar Parashar

7. The Reaction Mechanism and Reagents in Organic Chemistry, Chatwal, 5thEdn, Himalaya, 2008. 7

8. Organic Chemistry, R.T. Morrison and R.N. Boyd, 7thEdn, Prentice Hall, New Delhi, 2005.

9. Advanced Organic Chemistry, R.A. Carey and R.J. Sundberg, 5thEdn, Plenum, New York, 2008.

10. A Text book of Organic Chemistry, R.K. Bansal, 5thEdn, New Age, New Delhi, 2006.

11. Organic Chemistry, I.L. Finar (Vol I and II), ELBS, England, 1997.

PH 583.1: PHYSICAL CHEMISTRY

Course Outcome:

Student will be able to:

- Understand the basic concepts of thermodynamics and its applications.
- Recollect the basics and understand fundamental ideas of chemical kinetics and its applications
- Familiarize with the various concepts in heterogeneous catalysis.
- Study and apply the principle and applications of electrochemistry

UNIT – I : **14 hours**

Concept of Entropy, Enthalpy and Free energy (Gibb's and Helmholtz).A brief resume of laws of thermodynamics (combined form of 1st and 2nd laws), entropy as a measure of unavailable energy.

Chemical Thermodynamics: Concept of fugacity and free energy, entropy and free energy changes and spontaneity of processes. Variation of free energy with T & P, Maxwell's relations, thermodynamics equations of state, limitations of Van't Hoff's equation, Nernst heat theorem & its applications. Third law of thermodynamics, determination of third law of entropies.

Application of thermodynamics: Entropy and free energy of mixing, partial molar quantities, partial molar volume and free energy (chemical potential), their significance and determinations. Gibbs-Duhem and Duhem-Margules equations.

Thermodynamics of non-ideal solutions -Activity, activity coefficient-standard states.

Thermodynamics of ideal solutions - deductions of laws of Raoult's ebullioscopy, cryoscopy and osmotic pressure.

UNIT - II: **14 hours**

Rate of a reaction – definition, rate equations of simple chemical reactions, order of a reaction – definitions and units.

Chemical kinetics: Complex reactions- parallel, consecutive and reversible reactions. Branched chain reactions-general rate expression, explosion limits. Photochemical (hydrogen-halogen reactions) and oscillatory reactions.

Reactions in solution: Ionic reactions- salt and solvent effects. Substituent effects on the rates of reactions-Hammett and Taft equations.

Theories of reaction rates: Collision theory, activated complex theory and its applications to reactions in solution. Lindemann's theory of unimolecular reactions, Hinshelwood treatment, Study of fast reactions. Flow method, Flash photolysis

UNIT-III **14 hours**

Homogeneous and heterogeneous catalysis, review of adsorption terms, Industrial application of catalysts.

Catalysis: Homogeneous catalysis-equilibrium and steady state treatments, activation energies of catalysed reactions. Acid-base catalysis (general and specific), protolytic and prototropic mechanisms, catalytic activity and acid strength measurements. Kinetics of enzyme catalysed reactions-Michaelis-Menten equation. Effect of pH, temperature & inhibitors

Surface reaction kinetics: A review of adsorption isotherms, uni- and bi-molecular reactions. Multilayer adsorption-BET equation-its derivation and application in surface area determination. Harkin`s–Jura equation and its application. Adsorption from solution, Gibbs adsorption, Desorption and heterogeneous catalysis – catalytic activity at surfaces, semiconductor catalysis, n-&p-type.Mechanism of surface reactions.

UNIT-IV **14 hours**

Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes

Electrochemistry of solutions: Nernst equation, Kohlrausch law of independent migration of ions. Activities in electrolytic solutions, mean activity coefficient Ionic atmosphere, Debye-Huckel-Onsager equation of conductivity and its validity. Walden`s rule and its application. Conductance minima, Concept of Ionic strength, Debye-Huckel limiting law (DHL), modifications to DHL-Types, qualitative tests and verification of DHL. Bjerrum theory of ion association-triple ion and significance.

Phase Rule: Concepts of phase rule, Application to two component system-simple eutectic system-Ag/Pb system and Zn/ Cd system. Three component systems, water-chloroform- acetic acid system, triangular plots.

REFERENCES :

1. Physical Chemistry, A W Atkins, 9thEdn, ELBS, 2009.

2. Physical chemistry, G. M. Barrow, 5thEdn, McGraw Hill, Int. St. Ed, 2002.

3.Fundamentals of Physical Chemistry, Maron and Lando, Collier Macmillan, 1974.

4. Thermodynamics for Chemists, S. Glasstone, East-west, 2007.

5. Chemical Kinetics, K.J.Laidler, 3rdEdn, Harper and Row, 2003.

6. Electrochemistry, S. Glasstone, 1stEdn, Affiliated to East-west press, 2006.

7. Principles and Applications of Electrochemistry, Crow & Crow, 4thEdn, Chapman hall, London, 2004

8. Modern electrochemistry - vol I 2A&2B, Bockris and Reddy, 2ndEdn, Plenum, New York, 1998.

9. Advanced Physical Chemistry, Gurudeep Raj, 35thEdn, Goel Publishing House, 2009.

10. Chemical Kinetics and Reaction Dynamics, Santhosh Upadhyay, 1stEdn, Springer, 2010.

11. Principles of Physical Chemistry, Puri and Sharma, 47thEdn, Vishal Publishing House 2016

PS 584.1 : PRINCIPLES OF ANALYTICAL CHEMISTRY & SEPARATION TECHNIQUES

Course Outcome:

Student will be able to:

- Imbibe knowledge about various sampling techniques and errors.
- Evoke the fundamental concepts of different titration techniques
- Understand the principle of different chromatography techniques and apply that knowledge for the separation and purification of various samples

UNIT- I: **14 hours**

Types of errors- Determinate and indeterminate errors. Accuracy and precision. Introduction to gravimetric analysis

Distribution of random errors- frequency distribution, the normal error curve. Statistical treatment of finite samples. Measures of central tendency- mean, median, mode, range, average deviation, relative average deviation, standard deviation and variance. Student's t test, confidence interval of the mean. Testing for significance, comparison of two means and two standard deviations. Criteria for rejection of an observation-Q test. Principles of sampling- The sampling steps. Methods for sampling solid, liquid and gaseous samples. Effects of sampling uncertainties. Sampling hazards.

Gravimetry: Precipitation methods, the colloidal state, Super saturation and precipitate formation., purity of the precipitate: co-precipitation, post-precipitation, Conditions for precipitation, precipitation from homogeneous solution, washing the precipitate. Fractional precipitation, organic precipitants.

UNIT-II **14 hours**

Stability of complexes, stepwise and overall stability constant

Acid base titrations: Titration curves for strong acid-strong base, weak acid-strong base and weak base-strong acid titrations. Polyprotic acids, poly equivalent bases. Determining the equivalence point-theory of acid-base indicator, colour change range of indicator, selection of proper indicator. Typical applications of acid-base titrations.

Redox titrations: Equilibrium constants for redox reactions - electrode potentials in equilibrium systems, calculation of equilibrium constants. Redox titration curves- formal potentials, derivation of titration curves. Factors affecting the shape of titration curves- concentration, completeness of reaction. Titration of mixtures- feasibility of redox titrations. Detections of end point -redox indicators, theory, specific and non specific indicators, choice of indicator, potentiometric end point detection. Karl Fischer reagent for water determination. Applications

Complexometric titrations: Complex formation reactions, chelating agents. EDTA-acidic properties, complexes with metal ions, equilibrium calculations involving EDTA, conditional formation constants, derivation of EDTA titration curves, effect of other complexing agents, factors affecting the shape of titration curves. Completeness of reaction, indicators for EDTA titrations, theory of common indicators. Titration methods employing EDTA-direct, back and displacement titrations, indirect determinations. Titration of mixtures, selectivity, masking and demasking agents, Typical applications of EDTA titrations- magnesium, manganese and zinc in a mixture. Titrations involving unidenate ligands-titration of chloride with Hg^{2+} and cyanide with Ag^{+}.

UNIT III: **14 hours**

Basic Concepts - General description, Classification of chromatographic methods. Rf value and factors affecting Rf values.

Solvent Extraction: Definition, types, principle and efficiency of extraction. Sequence of extraction process. Factors affecting extraction-pH, oxidation state, modifiers, synergistic, masking and salting out agents. Techniques-batch and continuous extraction, Application.

Column Chromatography - High Pressure Liquid Chromatography (HPLC): Principle, instrumentation Apparatus, pumps, types of columns, packing and characteristics of liquid chromatographic detectors-UV, IR detectors. Advantages and applications, LC-MS.

Ion-exchange Chromatography (IEC): Synthesis and types of ion-exchange resins. Principle, factors affecting ion-exchange equilibria. Resin properties- ion-exchange capacity Applications of IEC in preparative, purification and recovery processes.

Gas Chromatography (GC): Principle, comparison of GSC and GLC. Instrumentation, Columns-packed and tubular. Study of detectors- thermal conductivity, flame ionization, electron capture, GC-MS. Factors affecting separation, applications.

REFERENCES

1. Comprehensive Analytical Chemistry, Lobinski and Marczenko, Vol.30, Elsevier, 1996.
2. Chromatography, E. Heftman (Ed), Part A and Part B, 5thEdn. Elsevier, 2004.
3. Fundamentals of Analytical Chemistry, S.A. Skoog, West & Holler, 9thEdn, Cengage, 2014.
4. Principles of Instrumental Analysis, Skoog, Holler and Nieman, 6thEdn. Saunders, 2006.
5. Quantitative Analysis, R. A. Day and A. L. Underwood, 6thEdn, Prentice-Hall, 2008.
6. Instrumental Methods of Chemical Analysis, B. K. Sharma, 1stEdn, Goel, 2012.
7. Vogel's Text book of Quantitative Inorganic Analysis, Bessett, Denney, Jeffery &Mendham, 5thEdn, 1989.
8. Instrumental methods of Chemical Analysis, Gurudeep.R.Chatwal, S Chand, 2010.
9. Non-aqueous titrations-Waiter Huber, Academic Press, 1987.
10. Instrumental methods of analysis, Gray Calvin and Bhatia, 1stEdn, 2009.
11. Introduction to Instrumental analysis, Robert D Braun, BSP Books, 2012.
12. Instrumental Methods of Analysis, Willard, Merritt and Dean Settle, 7thEdn, 2012.
13. Instrumental Methods of Analysis, H Kaur, Pragathi Prakashan, 2012.
14. Analytical Chemistry, G D Christian, 6thEdn, Wiley, 2007.

PS 585.1 BIO-ORGANIC CHEMISTRY

Course Outcome:

Student will be able to:

- Understand the chemical principles of living cells, the biomolecules and biocatalytic reactions.
- Study the basic principles underlying the chemistry of nucleic acids.
- Explain the structure determination, synthesis and classification of biomolecules like vitamins and lipids

UNIT I : **14 Hours**

Classification of amino acids based on structure, nature and biological importance. Properties such as isoelectric point, zwitter ion nature and amphoteric nature.

Amino acids and peptides: Introduction and synthesis of amino acids, structure and conformation of peptide bond, N-terminal, C-terminal. Determination of peptides, enzymic cleavage of peptides, reagents for selective cleavage of polypeptide bonds.**Peptide synthesis:** Solution phase and Merrifield's solid phase synthesis, solution phase synthesis of oxytocin and vasopressin.

Proteins: Classification, structural detrmination: Primary, secondary, tertiary and quarternary. Stereochemistry of peptide chains, chemical bond involved in protein structure. Protein confuguration: α-helix, amino acids effecting α-helix, rigid and planar peptide bond, Ramachandran plot, β pleated sheets, structure of silk fibroin, random coil structure of proteins, triple helical structure of collagen, similarity in 3D structure of haemoglobin and Myoglobin.

UNIT II : **14 Hours**

Types of nucleic acids, differences between DNA & RNA both in structure and biological functions

Nucleic acids : Introduction, nucleosides and nucleotides, structure of nucleoside, chemical synthesis of nucleoside- Adenosine, Guanosine(purine nucleosides), structure of nucleotide, synthesis of nucleotide(AMP). DNA(Watson-Crick model of double stranded DNA) and RNA. Functions of nucleic acids : Replication, transcription, translation, protein synthesis, flow of genetic information, genetic code.

UNIT III : **14 Hours**

Introduction, classification and nomenclature- source and deficiency diseases-biological functions of vitamins

Vitamins:. Study of following vitamins: Vitamin A_1& A_2, Vitamin B_1, B_2, B_6&B_{12}, Vitamin C, Vitamin D_2& D_3, Vitamin K_1& K_2, pantothenic acid, folic acid.

Lipids : Introduction, classification of lipids, synthesis of fatty acids. Compound lipids-Phospholipids, Glyco, spingo lipids and derivatives.

REFERENCES :

1. Lehninger's Principles of Biochemistry - Nelson & David, 6th Edn, MacMillan, 2013.
2. Harper's Illustrated Biochemistry-Bender, Kennelly &Rodwell, 30thEdn, McGraw Hill, 2015.
3. Text Book of Medical Biochemistry - Chatterjea&Shinde, 8thEdn, JayPee Brothers Medical Publications, 2011.
4. Bioorganic Chemistry - Hermann Dugas, 3rdEdn, Springer New York, 1999.
5. Fundamentals of Biochemistry-Vol 1&2, J L Jain, S Chand & Company Ltd, 2005.
6. Amino acids and Peptides- G C Barret and D T Elmore, Cambridge University Press,1998.
7. The Carbohydrates - Vol. IA, IB, IIA and IIB- W Pigman and D Horton, Academic Press, 1970.

PS 586.1 RESEARCH METHODOLY

Course Outcome

Student will be able to:

Evaluate Research output with philosophical base and greater relevance to the society

Identify the parameters of Quality research with scientific methodology

Understand the concepts involved in Original Research, ethical guidelines and practices in conducting the research and publication of papers.

Create awareness on Intellectual property Rights and Patents.

Unit 1: Foundation of Research and Research Methodology: 14 Hours

Research – meaning, characteristics, objectives, motivation in research, need and importance of research. Types of Research; Philosophy and Research Philosophy – Ontology, Epistemology, Axiology, positivism, critical realism, interpretivism, post modernism, pragmatism – meaning, relevance and assumptions. Concept of Theory and Theory Building – deduction, induction and abduction. Research Strategies - meaning and types.

Research Problem – meaning, selecting the problem, sources of problem, statement of a problem;

Review of Literature – meaning and need for literature review, sources of literature review, reporting the review of literature, identification of research gap; Print : Sources of information – Primary, Secondary, Tertiary sources – Journals – Journal abbreviations – Abstracts – Current titles – Reviews – Monographs – Dictionaries – Textbooks – Current contents – Introduction to Chemical Abstracts and Beilstein – Subject Index, Substance Index, Author Index, Formula Index and other Indices with examples. Digital : Web resources – E–Journal – Journal access – TOC alerts – Hot articles – Citation index – Impact factor – H–Index – E–Consortium – UGC infonet – E–Books – Internet discussion groups and communities – Blogs – Preprint server – Search engines, Scirus, Google Scholar, ChemIndustry, Wiki – Databases, ChemSpider, ScienceDirect, SciFinder, Scopus.

Unit 2 : Chemical Safety and Ethical Handling of Chemicals 14 hours

Safe working procedure and protective environment, protective apparel, emergency procedure and first aid, laboratory ventilation, Safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at above or below atmospheric pressures – safe storage and disposal of waste chemicals , recovery , recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives , identification , verification and segregation of laboratory waste , disposal of chemicals in the sanitary sewage system , incineration and transportation of hazardous chemicals .

Unit 3: Research Ethics and Intellectual Property Rights (IPR): (14 Hours)

Ethics – meaning and definition, Ethics Vs moral philosophy, nature of moral judgments and reactions. Rights and obligations of Research Participants. Scientific conduct – ethics with respect to science and research, intellectual honesty and research integrity. Scientific misconduct – falsification, fabrication and plagiarism. Publication ethics – meaning and importance, plagiarism and Self-plagiarism

IPR – Concept of IPR, nature and characteristics of IPR, origin and development of IPR, justification and rationale for protecting IPR, IPR and sustainable development, IPR and human rights,. Forms of IPR – copyrights, trademarks, patents, industrial designs, trade secrets, geographical indications – meaning, features and application of different forms of IPRs. Filing and Registration process of IPRs.

References:

1. Indian National Science Academy (INSA). (2019). Ethics in Science Education, Research & Governance

2. Barbara H Stanley J Joan E Sieber, Gary B Melton. Research Ethics: A Psychological Approach. University of Nebraska Press

3. David I Bainbridge (2012), Intellectual Property Rights. Long man Publication

4. Jayashree Watal. Intellectual Property Rights in the WTO and Developing Countries. Oxford University Press

5. A K Singh. Tests, Measurements and Research Methods in Behavioral Sciences. Bharathi Bhawan (Publishers & Distributors), New Delhi

6. Leedy P D. Practical Research: Planning & Design. Washington: Mc Millan Publishing Co., INC

7. Singh Y K. Fundamentals of Research Methodology and Statistics. New International (P) Ltd., New Delhi.

8. Wallinman N. Your Research Project: A Step by Step Guide for the first time Researcher. Sage Publications, London

9. Kothari C R. Research methodology: Research & Techniques. New Age International Publishers, New Delhi

10. Chemical safety matters–IUPAC –IPCS, Cambridge Univ. Press, 1992

PS 587.1P : INORGANIC CHEMISTRY PRACTICALS – I

Course Outcome:

Student will be able to:

- Estimate the quantity and quality of different compounds and metal ions using gravimetry, volumetry and complexometric techniques.

Any 10 experiments are to be carried out

1. Analysis of Hematite-insoluble residue by gravimetry and Iron by volumetry using Ce^{4+}.
2. Analysis of Dolomite- insoluble residue by gravimetry and Ca, Mg by complexometry.
3. Pyrolusite- Insoluble residue by gravimetry and Manganese content by oxalate method.
4. Complexometric determination of Mn, Cu.
5. Complexometric determination of Ni and Fe-Cr mixture
6. Hardness of water
7. Analysis of Halide Mixture - Iodide by KIO_3 and total halide by gravimetry.
8. Colorimetric Determination of Iron by thiocyanate and Cu by aqueous ammonia.
9. Gravimetric Determinations of Mn, Ni.
10. Analysis of solder - Pb and Sn by EDTA method.
11. Gravimetric Determinations of Mo, Pb/Cr, sulphide, thiocyanate.
12. Estimation of Cr(III) & Fe(III) in a mixture using EDTA.
13. Estimation of Ni(II) & Fe(III) in a mixture using EDTA.
14. Determination of free Chlorine in the given water sample
15. Any other experiment of interest

REFERENCES :

1. Vogel's Text Book of Quantitative Chemical Analysis, G.H.Jeffrey, J.Bassette, J.Mendham and R.C.Denny, 6thEdn, Longman, 2009.

PS 588.1P : ORGANIC CHEMISTRY PRACTICALS - I

Course Outcome:

Student will be able to:

- Carry out multi-step organic synthesis
- Purify the synthesized organic compounds

Any 10 experiments are to be carried out

1. Electrophilic substitution reactions–Preparations of p-bromoaniline, p-nitroaniline and picric acid
2. Alkylations–Preparations of nerolin and N-methyl anthranilic acid.
3. Acetylations–Preparations of β-D-glucose penta-acetate and 2-naphthyl acetate.
4. Reactions with ring formation–Preparations of 1,2,3,4–tetrahydrocarbazole and 7– hydroxy-4-methyl-coumarin.
5. Diazotisation reactions–Preparations of iodo, chloro and azo compounds.
6. Dehydration reactions–Preparations of cyclohexene and succinic anhydride
7. Condensation reactions–Condensations involving diethylmalonate and ethyl acetoacetate. Aldol condensation and Perkin reactions.
8. Oxidation reactions-Preparation of p-nitrobenzoic acid and adipic acid.
9. Halogenation reactions-Preparation of n-butylbromide &α,β-dibromocinnamic acid.
10. Oxidation reactions–Preparation of adipic & p-nitrobenzoic acids and p- benzoquinone.
11. Reduction reactions–Reductions of nitro compounds and carbonyl compounds.
12. Preparation of Dibenzal Acetone.
13. Preparation of Cinnamic Acid from Benzaldehyde.
14. Preparation of Ethyl Aceto Acetate from Ethyl acetate.
15. Any other experiment of interest

REFERENCES :

1. Laboratory Manual in Organic Chemistry, R. K. Bansal, 5thEdn, New Age, New Delhi, 2008.
2. Experimental Organic Chemistry–Vol. I & II, P. R. Singh et al, TMH New Delhi, 2013.
3. Vogel's Text Book of Practical Organic Chemistry including Qualitative Organic Analysis, B. S. Furniss et al, 2ndEdn, Longman-ELBS, London, 1989.
4. Practical Organic Chemistry, F G Mann, 4thEdn, Pearson Education, 2009.

PS 589.1P : PHYSICAL CHEMISTRY PRACTICALS – I

Course Outcome:

Student will be able to:

- Carry out experiments related to chemical kinetics, viscometry, Polarimetry, Refractometry, Conductometry and Potentiometry

Any 10 experiments are to be carried out

1. Potentiometric titration of halides in mixtures (Cl^-, Br^- and I^-) with silver nitrate
2. Potentiometric determination of redox potentials.
3. Potentiometric determination of dissociation constants of weak acids
4. Potentiometric and conductometric acid–base titrations in partial & non-aqueous media.
5. Conductometric titrations of displacement and precipitation reactions
6. Determination of equivalent conductances and dissociation constants of weak acids.
7. Determination of solubility of lead iodide at different T & hence molar heat of solution
8. Determination of pH of buffer solutions with a pH meter & evaluation of pKa of acids
9. Analysis of a binary mixture and determination of molar refraction of a solid and the composition of chloroform and acetone in its azeotropic mixture by refractometry
10. Analysis of a binary mixture of two miscible liquids by viscometry and the relation between viscosity of a solution and the electrical conductivity
11. Study of variation of viscosity of a liquid with temperature
12. Determination of parachor value for CH_2 group by S.T method, the composition of asolution by S.T measurement and the CMC of a soap solution by S.T measurement.
13. Potentiometric determination of solubility of insoluble silver halide and the standard electrode potential using quinhydrone electrode
14. Determination of degree of hydrolysis of CH_3COONa and NH_4Cl.
15. Determination of hydrolysis constant of aniline hydrochloride.
16. Verification of Nernst equation for Ag^+, $Cu^{2+}$and Zn^{2+} species.
17. Determination of transport number of ions by emf method (Ag^+, Cd^{2+}, NO^-_3, SO_4^{2-} etc.)
18. Any other experiment of interest

REFERENCES :

1. Findlay's Practical Physical Chemistry, B. P. Levitt, Longman, London, 2010.
2. Experiments in Physical Chemistry, Carl W. Garland , Joseph W. Nibler , David P. Shoemaker, 8th Edn, Tata McGraw - Hill Education, 2008.
3. Experimental Physical Chemistry, Daniels et al, Nabu Press, 2011.
4. Experimental Physical Chemistry, Das&Behera, Tata-McGraw Hill, New Delhi,1984.
5. Advanced Practical Physical Chemistry, Yadav, 33rd Edn, Krishna Prakashan, 2013.
6. Experiments in Physical Chemistry, Carl, Joseph, David, 8th Edn, Tata-McGraw Hill, 2008.

SECOND SEMESTER

PH 581.2: ADVANCED INORGANIC CHEMISTRY

Course Outcome:

Student will be able to:

- Understand the Chemistry of d block elements, Lanthanides and Actinides and explain their magnetic and electronic properties
- Describe the VB and MO theory of complexes and electronic and bonding reactivities of transition metals
- Explain the spectral and magnetic properties of metal complexes
- Describe the basic concepts of organometallic chemistry and their bonding patterns especially with unsaturated ligands

UNIT I: **14 Hours**

Definition of metallurgy - roasting and calcination, reduction of mineral to metal (electrolytic reduction, chemical reduction and auto reduction), General characteristics of d and f block elements, lanthanide and actinide contraction.

Reduction of Ores: Methods of reduction of oxide ores Ellingham diagram, chemical and electrolytic reductions, reduction potentials, Latimer and Frost diagrams, Pourbaix diagram, effect of complexation on potential.

d block elements: Comparison of 3d, 4d and 5d series by taking Titanium subgroup as example.

Lanthanides and actinides: extraction and separation of lanthanides, spectral and magnetic properties of lanthanide and actinide complexes, lanthanide and actinide contraction Comparison of spectral and magnetic properties of lanthanides and actinides with d-block ions.

UNIT II: **14 Hours**

Review of basic concepts of co-ordination chemistry, Valence bond and Crystal field theories, Concept of hybridization coordination number and geometry in coordination compounds. Stepwise and overall formation constants, factors affecting stability of metal complexes.

Complexes with Coordination numbers 2-10 and their geometry, crystal field theory of coordination compounds, d-orbital splittings in octahedral, square planar and tetrahedral fields, spectrochemical series, Jahn-Teller effect.

Evidences for ligand field splitting: hydration, ligation and lattice energies, site preference energies. Metal – ligand orbital overlap from ESR, NMR, electronic spectra and antiferromagnetic coupling, nephelauxetic effect and nephelauxetic series, MO theory of coordination compounds-MO energy level diagrams for octahedral, tetrahedral and square planar complexes.

Determination of composition and stability constants of complexes by spectrophotometry (Job's method) and potentiometry, stepwise stability constants by Bjerrum's pH-titration method, Rossotti and Rossotti method, Bjerrum's spectrophotometric method and ion exchange method

UNIT III: **14 Hours**

Concept of pi acceptor ligands, back bonding, bonding in metal carbonyls, 18 electron rule

Metal Pi-acceptor complexes: Metal carbonyls – preparative methods, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, magnetic and X-ray evidences of structures. Reactions of metal carbonyls. Metal carbonylates and carbonyl halides – preparation and important reactions with Applications. Chemistry of metal nitrosyls – preparation, structure and bonding; dinitrogen and tertiary phosphine complexes, ligand cone angle in phosphine complexes, complexes containing SO_2 and CO_2

Metal complexes as liquid crystals: Stereochemical non-rigidity, Stereoisomeriosm – chirality, optical activity, CD, ORD, Cotton effect

Metal-metal bonding in carbonyls and halides: Evidences for M-M bonding, factors favouring M-M bond formation.

UNIT IV: **14 Hours**

Quantum numbers and their significance. Brief review of different types of magnetic behaviour

Electronic spectra of transition metal complexes: Spectroscopic term symbols for d^n ions, ground states, microstates, microstate table for p^2 and d^2 system. selection rules, Racah parameters, Orgel, Tanabe-Sugano diagrams, spectra of 3d metal aqua complexes of trivalent, V, Cr, divalent Mn, Co and Ni, $[CoCl_4]^{2-}$, calculation of Dq, B and β parameters, charge transfer spectra.

Magnetic properties of metal complexes: Origin and types of magnetic behaviour- diamagnetism, paramagnetism, ferro and antiferromagnetism, magnetic susceptibility and its measurement by the Guoy method, temperature dependence of magnetism – Curie and Curie-Weiss laws, Curie Temperature and Neil temperature, types of paramagnetic behaviour, spin only behaviour, spin orbit coupling, quenching of orbital contribution and spin only behaviour (explanation based on A, E and T terms), application of magnetic data.

REFERENCES:

1. Inorganic Chemistry, J.E Huheey, E.A..Keiter, R.L.Keiter and O K Medhi, 4th Edn,Pearson Education, 2006.
2. Inorganic Chemistry, Shriver, Atkins and Langford, 5th Edn, Oxford, 2009.
3. Concise Inorganic Chemistry, J.D.Lee,, 5th Edn, Blackwell Science, 2014.
4. Concepts and Models of Inorganic Chemistry, B.E.Douglas, D.McDaniel and A Alexander, 3rd Edn, Wiley, 2010.
5. Inorganic Chemistry, A Unified Approach, W.W. Porterfield, 2nd Edn, Elsevier, 2009.
6. Principles of Inorganic Chemistry, Puri, Sharma and Kalia, 33rd Edn, Vishal Publishing House, 2016.
7. Selected Topics in Inorganic Chemistry, Madan, Malik and Tuli, 17th Edn, S Chand, 2010.
8. Inorganic Chemistry, Meissler and Tarr, 5th Edn, Pearson Prentice Hall, 2013.

PH 582.2: ADVANCED ORGANIC CHEMISTRY

Course Outcome:

Student will be able to:

- Describe the mechanisms of different types organic reactions.
- Understand the chemistry of radical reactions and its applications.
- Understand the mechanism of additions to various Carbon-based multiple bonds
- Achieve skills in constructing homo/heterocyclic rings of significant molecules

UNIT I **14 hours**

Generation of Nucleophiles and electrophiles, electrophilic and Nucleophilic substitution reactions.

Aliphatic Nucleophilic Substitution Reactions: Mechanism and scope of aliphatic nucleophilic substitution reactions - S_N1, S_N2 and S_Ni. Stereochemistry of nucleophilic substitution reactions, allylic, vinylic and benzylic nucleophilic substitution reactions, neighbouring group participation and anchimeric assistance.Factors influencing the rates of nucleophilic substitution reactions.

Aliphatic Electrophilic Substitution Reactions: Bimolecular mechanisms-S_E1, S_E2 and S_Ei mechanism. Electrophilic substitution reactions accompanied by double bond shifts.

Aromatic Electrophilic and Nucleophilic Substitution Reactions: Mechanism of aromatic electrophilic substitution reaction pathway, Arenium ion mechanism, orientation and reactivity, energy profile diagram. The ortho/para ratio, ipso attack, orientation in other ring systems.Mechanism of Mannich Reaction.

Mechanisms of aromatic nucleophilic substitution reactions:SNAr, SN1 and aryne mechanism. Von-Richter rearrangement, Sommelet-Houser rearrangement, Smiles rearrangement.

UNIT II **14 hours**

Elimination reactions, dehydration, dehydrohalogentation and dehalogenation

Free Radical Reactions: Types of radical reactions, mechanisms of free radical substitution reactions and neighbouring group assistance. Reactivity for the aliphatic and aromatic substances at a bridgehead.Reactivity of the attacking radical.The effect of solvent on reactivity.Auto-oxidation, coupling of alkynes.Arylation of aromatic compounds by diazonium salts. Sandmeyer, Ullmann and Hunsdiecker reaction

Elimination Reactions: Discussions of E1, E2, E1cB and E2cB mechanisms. Orientation during elimination reactions.Saytzeff and Hofmann rules.Reactivity-effects of substrate structures, attacking base, leaving group and solvent medium.

Pyrolytic Eliminations: Mechanisms of pyrolysis of esters of carboxylic acids, (acetate pyrolysis), Chugaev reaction, Hofmann degradation and Cope elimination

UNIT III **14 hours**

Addition and condensation reactions, aldol condensation and Perkin reaction

Formation and Hydrolysis of Esters: Plurality of mechanism. Mechanism of esterification reactions.Ester hydrolysis-$A_{AC}2$, $B_{AC}2$, $A_{AC}1$ & $A_{AL}1$ mechanism. Transesterification – acetyl and benzoyl migrations.

Addition to Carbon-Carbon Multiple Bonds: Addition reactions involving electrophiles, nucleophiles and free radicals. Cyclic mechanisms.Orientation and stereochemistry.Addition of halogens, hydrogen halides, carboxylic acids and amines.Addition to cyclopropanes, hydroboration, Michael addition.Addition of oxygen across double bonds.

Addition to Carbon-Hetero Multiple Bonds: Electrophilic, nucleophilic and free radical additions to C=O and C=N systems. Addition of Grignard reagents.Reformatsky reaction, Knoevenagel condensation and Wittig reactions.

UNIT IV **14 hours**

Introduction and classification of heterocycles

Chemistry of Heterocyclic Compounds: Nomenclatureof 3,4, 5, 6 membered heterocyclic and fused heterocycles, synthesis and reactions of oxiranes, thiranes, aziridenes, azirenes. Structure, synthesis and reactions of pyrrole, thiophene,furan.Synthesis and reactions ofpyridine, quinoline, isoquinoline, indole. Synthesis and reactivity of heterocycles containing two hetero atoms(pyrazole, imidazole, thiazole).

REFERENCES:

1. Organic Reactions and Their Mechanisms- P.S. Kalsi, 3rdEdn, New Age, New Delhi, 2010.
2. March's Advanced Organic Chemistry, Smith, 6thEdn, Wiley, NY, 2012.
3. Organic Reaction Mechanisms- Bansal, 4thEdn, Tata McGraw Hill, New Delhi, 2012.
4. Organic Chemistry-Vol. –I & II, Mukherji, Singh and Kapoor, 2ndEdn, Wiley Eastern, New Delhi, 2012.
5. The reaction mechanism and reagents in Organic Chemistry, Chatwal, 5thEdn, Himalaya, Bombay, 2010.
6. The Chemistry of Carbonyl Compounds, David Gutsche, Prentice-Hall, New Delhi, 1988.
7. An Introduction to the Chemistry of Heterocyclic Compounds, Acheson, 3rdEdn, Wiley – Eastern, 2008.
8. Heterocyclic Chemistry, J. Joule & G. Smith, 3rdEdn, Van-Nostrand, ELBS, 1995.
9. Organic Chemistry, Claydon and Greaves, 2ndEdn, 2012.
10. Advanced Organic Chemistry, Carey and Sundberg, 3rdEdn, 1990.
11. Organic Chemistry-Vol. –I & II, I.L. Finar, 6thEdn, Longman-ELBS, England, 2002.
12. Reaction Mechanisms in Organic Chemistry, Mukherji, Singh and Kapoor, 3rdEdn, McMillan, 1984.
13. Organic Chemistry, P.Y. Bruice, 7thEdn, Pearson Education, New Delhi, 2014.
14. Text Book of Heterocyclic Chemistry, R.K.Bansal, 5thEdn, 2010.
15. Heterocyclic Chemistry, J A Joule & K Mills, 5thEdn, Wiley-Blackwell, 2010.

PH 583.2: ADVANCED PHYSICAL CHEMISTRY

Course Outcome:

Student will be able to:

- Gather knowledge of Quantum Chemistry and its application
- Explain the approximation methods in quantum mechanics
- Explain the relationship between microscopic properties of molecules with macroscopic thermodynamic observables
- Describe the quantum mechanical explanation of chemical bonding

UNIT - I : **14 hours**

Bohr's theory of hydrogen atom. Comparison of classical and quantum mechanical particles. Cartesian, Polar and spherical polar coordinates and their interrelations. Operators, matrix representation and commutation relationships, Angular momenta (commutations, relations, operators). Schrödinger equation, significance and characteristics of wave function, eigen functions and eigen values. Probabilities, normalisation and orthogonality. Postulates of quantum mechanics ϕ, θ Solution of Schrödinger wave equation for exactly solvable problems such as particle in a box (1D and 3D), particle in a ring, harmonic oscillator, rigid rotor and hydrogen atom **(**separation of r,ϕ, θ equations and their solutions).

UNIT–II: **14 hours**

Pauli exclusion principle, Term symbols, Russell-Saunders terms and coupling schemes

Approximate methods in quantum chemistry: Approximate methods of solving Schroedinger equation for problems of chemical interest - variation and perturbation methods. Application of variation method to H & He atoms, the structure of many electron systems/atoms (secular equations & determinants). Spin-orbit interaction, antisymmetry, Slater orbitals and SCF method for many electron systems.

Molecular wave functions: Born-Oppenheimer approximations. Covalent bond –valence bond and molecular orbital approaches with comparisons. Hydrogen molecule – Heitler-London (VB) treatment. Energy level diagram. MO theory applied to homonuclear and heteronuclear diatomics by LCAO methods, correlation diagrams, non-crossing rule.

UNIT -III : **14 hours**

Hybridization and Valence Bond Theory (VBT), Molecular Orbital Theory(MOT).

Theory of directed valence - Geometry of molecules in terms of molecular orbitals (bond angle, dihedral angle), localised and delocalised molecular orbitals.

Conjugated and aromatic molecules: Huckel molecular orbital (HMO) theory of linear conjugated systems (ethene, allyl & butadiene systems) and aromatic molecules (benzene as an example). Calculation of delocalization energies, bond order & charge density. An introduction to Extended Huckel Theory.

UNIT - IV : **14 hours**

Concept of molecular energy levels. Maxwell`s distribution of molecular velocities

Statistical Thermodynamics : Micro and macrostates, phase space and ensembles. Concept of distribution - thermodynamic probability and most probable distribution - Maxwell-Boltzmann distribution law. Maxwell-Boltzmann statistics and applications, Bose-Einstein and Fermi-Dirac statistics. Partition functions - definitions and separations, evaluation of translational, rotational, vibrational and electronic partition functions for monoatomic, diatomic and polyatomic gaseous molecules. Calculations of thermodynamic functions and equilibrium constant in terms of partition functions, entropy of monoatomic gas - Sackur-Tetrode equation, comparison of 3rd law and statistical entropies. Heat capacity behaviour of solids – Einstein and Debye theories. Introduction to Irreversible Thermodynamics

REFERENCES :

1. Physical Chemistry, P Atkins, 9th Edn, ELBS, 2009

2. Introductory Quantum Chemistry – A. K. Chandra, 4th Edn, Tata McGraw Hill,

2009.

3. Statistical Thermodynamics, M. C. Gupta, 2ndEdn, Wiley Eastern Ltd, 1991.

4. Quantum Chemistry, Donald Mcquarrie, 2ndEdn, 2011. Tata McGraw Hill.

5. Quantum Chemistry, R K Prasad, 4thEdn, 2020, New AGe.

6. Physical Chemistry, T. Engel and P. Reid, 1st Edn, Pearson Education 2006.

7. Principles of Physical Chemistry, Puri, Sharma and Pathania,1stEdn, 2008

8. Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill, 2nd Edn. 1990

9. Molecular Quantum Mechanics, P. W. Atkins & R. S. Friedman, Oxford University Press, 5th Edn. 2012

PS 584.2: MOLECULAR SYMMETRY AND MOLECULAR SPECTROSCOPY

Course Outcome:

Student will be able to:

- Apply the principles of group theory in chemical bonding.
- Define aspects of specific spectroscopic techniques, applications of molecular symmetry in Microwave and Vibrational spectroscopy
- Define aspects of specific spectroscopic techniques, applications of molecular symmetry in Rotational and Raman spectroscopy

UNIT – I : **14 hours**

Elements of Symmetry, Definitions of groups and sub groups, symmetry operations

Symmetry and Group Theory : Relation between orders of a finite group and its subgroup and group multiplication tables, Conjugate relationships and classes, Schoenflies symbols, Matrix representations of symmetry operations, products of symmetry operations, some properties of matrices and vectors, classification of molecules into point groups. Reducible and irreducible representations. Mulliken's symbols for IR's The Great Orthogonality theorem (without proof), character tables for C_{2v}, C_{3v}, and C_2 point groups, the direct product.Transformation properties of atomic orbitals.Applications of group theory to molecular vibrations and chemical bonding (IR &Raman).

UNIT – II : **14 hours**

Rigid rotator definition & derive $I=\mu r^2$. Electromagnetic radiation, dual nature, regions of the spectrum.

Unifying Principles: Interaction of electromagnetic radiation with matter - absorption, emission, transmission, reflection, refraction, dispersion, polarization and scattering. Natural line width and broadening, intensity of spectral lines

Microwave Spectroscopy: The rotation and classification of molecules, selection rules, rotation spectra of diatomic and polyatomic molecules.Rigid and non-rigid rotator models.Determination of bond lengths, isotope effect on rotation spectra. Stark effect, nuclear and electron spin interaction. Microwave Spectrometer.

Vibrational Spectroscopy: Vibration spectra of diatomic molecules - linear harmonic oscillator, vibrational energies, zero point energy, force constants and bond strengths, anharmonicity of molecular vibrations - Morse potential energy diagram, selection rules, fundamental, overtones and hot bands. Vibrations of polyatomic molecules - normal modes of vibrations and nature of molecular vibrations (Ex - CO_2 and H_2O).

UNIT –III : **14 hours**

Introduction to Raman Spectroscopy, Stokes and Anti Stokes lines.

Vibration-rotation spectra of diatomic and polyatomic molecules, selection rules, PQR branches. IR Spectrophotometer-Instrumentation, sample handling techniques, FTIR Spectroscopy - Instrumentation

Raman Spectroscopy: Classical and quantum theories of Raman effect, concept of polarizability and polarizability ellipsoid. Rotational and vibrational Raman spectra, selection rules, Raman activity of vibrations, mutual exclusion principle, polarization of Raman lines.An introduction to Laser Raman Spectroscopy.Raman Spectrometer – instrumentation.Applications of IR and Raman spectroscopy in elucidation of molecular structure (Ex - H_2O, N_2O & CO_2 molecules).An introduction to Resonance Raman Spectroscopy.Advantages of Raman spectroscopy over IR spectroscopy.

REFERENCES:

1. Fundamentals of Molecular Spectroscopy, Banwell & McCash, 5thEdn, Tata McGraw Hill, 2015.

2. Organic Spectroscopy, W.Kemp, 3rdEdn, Mac, 2011.

3. Spectrometric Identification of Organic Compounds, Silverstein, Bassler&Monnill, 6thEdn, Wiley, 2010.

4. Elementary organic spectroscopy, Y R Sharma, 5thEdn, S Chand, 2013.

5. Introduction to Spectroscopy by Donald L. Pavia, Gary M. Lampman, George S. Kriz, James A. Vyvyan, 42ndEdn, 2008.

6. Spectroscopy of Organic Compounds, P. S. Kalsi, 6thEdn, 2004.

7. Organic Structures from Spectra, L D field, 5thEdn, 2013.

8. Symmetry and Spectroscopy of molecules, K Veera Reddy, 2ndEdn, 2010.

PS 585.2 : CHEMISTRY OF BIOMOLECULES

Course Outcome:

Student will be able to:

- Explain the structure and role of biomolecules like peptide, proteins and lipids
- Understand the chemical principles of living cells, their biomolecules and biocatalytic reactions.
- Detail the synthesis and stereochemistry of carbohydrates

UNIT I : **14 Hours**

Cell Structure and Functions: Structure of prokaryotic and eukaryotic cells, intra cellular organelles and anabolism, comparison of animal and plant cells

Overview of metabolic processes- catabolism and anabolism. ATP- the biological energy currency. Origin of life - unique properties of carbon, chemical evolution and rise of living systems.

Lipids: Fatty acids, essential fatty acids, structure and function of triglycerides, glycerophospholipids, sphingolipids, cholesterol, bile acids, prostaglandins.

Lipoprotiens: Composition and function, role in atherosclerosis, properties of lipid aggregates, micelles, bilayers, liposomes and their biological functions. Biological membranes-Fluid mosiac model of membrane structure. Lipid metabolism (oxidation of fatty acids).

UNIT II : **14 Hours**

General structure, classification, D and L Notation.

Amino Acids : Specific rotation, distribution in proteins, location in proteins, physical properties, non-standard protein aminoacids and non-protein aminoacids. General methods of synthesis of synthesis of aminoacids with specific examples.

Steriods and Hormones: Classification of steriods, Biological importance, Cholesterol, Occurance, properties, test and physiological activities of cholesterol. Sex hormones, thyroid gland hormones and adrenal gland hormones.

Enzymes: Enzymes in organic synthesis, α-carboxy peptidase-A and Ribonuclease. Enzymatic synthesis of α-amino acids and peptides. Transformations of lipases and esterases. Kinetic resolutions of carboxylic acids, esters and alcohols-Trans esterification. Enzymatic synthesis of α-amino acids and peptides.

UNIT III : **14 Hours**

Introduction, Definition, classification, reducing and non reducing sugars.

Carbohydrates : Configuration and conformation of monosaccharides, Chemistry of important derivatives of monosaccharides - ethers, esters, acetals, ketals, deoxysugars, aminosugars, structure of disaccharides - maltose, cellobiose and sucrose. Structure of tri and tetra saccharides.

General methods of structural degradation of polysaccharides-methylation, partial hydrolysis, per iodate oxidation, Smith degradation and alkaline degradation techniques. Structures of cellulose, chitin, starch(Amylose and amylopectin), glycogen, heparin and chondroitin. Hemicelluloses, regenerated cellulose and cellulose derivatives.

REFERENCES :

1. Lehninger's Principles of Biochemistry - Nelson & David, 6thEdn, MacMillan, 2013.
2. Harper's Illustrated Biochemistry-Bender, Kennelly & Rodwell, 30thEdn, Mc Graw Hill, 2015.
3. Text Book of Medical Biochemistry - Chatterjea & Shinde, 8thEdn, JayPee Brothers Medical Publications, 2011.
4. Biorganic Chemistry - Hermann Dugas, 3rdEdn, Springer New York, 1999.
5. Fundamentals of Biochemistry-Vol 1&2, J L Jain, S Chand & Company Ltd, 2005.
6. Amino acids and Peptides- G C Barret and D T Elmore, Cambridge University Press,1998.
7. The Carbohydrates - Vol. IA, IB, IIA and IIB- W Pigman and D Horton, Academic Press, 1970.

PS 586.2P : INORGANIC CHEMISTRY PRACTICALS – II

Course Outcome:

Student will be able to:

- Estimate binary mixtures of metallic ions in solution
- Analyse the presence of inorganic salts qualitatively

Qualitative Analysis of mixtures of Inorganic Salts containing 3 metal ions and 2 anions (1 less common metal ions like Tl, W, Mo, V, Zr, Th, U, Ce, Ti and Li to be included among anions organic acid radicals, phosphate, borate and fluoride separation included).

REFERENCES

1. Vogel's Text Book of Quantitative Chemical Analysis, G.H.Jeffrey, J.Bassette, J.Mendham and R.C.Denny, 6thEdn, Longman, 2009

2. Vogel's Qualitative Inorganic Analysis, G.Svehla,7thEdn, Longman, 2006.

PS 587.2P : ORGANIC CHEMISTRY PRACTICALS – II

Course Outcome:

Student will be able to:

- Separate and analyse the binary mixture of Organic Compounds

Separation and Systematic Qualitative Analysis of Binary Mixtures of Organic Compounds

REFERENCES :

1. Practical Organic Chemistry, F .G. Mann and B. C. Saunders, 4thEdn, ELBS, England, 2009.
2. Practical Organic Chemistry, A. I. Vogel, 5thEdn, Pearson India, 2005.
3. Laboratory Manual in Organic Chemistry, R.K. Bansal, 5thEdn. New Age Intl, 2008.
4. Experimental Organic Chemistry–Vol.I&II Singh et al, 1stEdn, Campus Books Intl, 2005.
5. The Systematic Identification of Organic Compounds– A Lab.Manual, R. L.Shriner, John Wiley & Sons, 6thEdn, 1980.
6. Vogel's Text Book of Practical Organic Chemistry, Furniss, 5thEdn, Pearson India, 2005.

PS 588.2P : PHYSICAL CHEMISTRY PRACTICALS – II

Course Outcome:

Student will be able to:

- Determine cryoscopic constants, dissociation constants and various other physical properties of compounds

At least 10 experiments are to be carried out

1. Determination of cryoscopic constants of solvents and molecular weight of non volatile substances using water and benzene as solvents.
2. Determination of degree of dissociation & Vant Hoff factor of an electrolyte by cryoscopic method.
3. Heat of solution of substances by solubility method.
4. Phase diagram of two component systems by thermal analysis.
5. Kinetics of acid catalysed hydrolysis of methyl acetate and determination of (a) order and rate constant, (b) Relative strength of two acids and (c) Energy of activation.
6. First and second order kinetics of reaction between potassium persulphate and KI.
7. Kinetics of (a) inversion of cane sugar, (b) sodium formate–iodine reaction .
8. Determination of heat of neutralisation, integral and differential heat of solution calorimetrically. Thermometric titration of an acid with a base.
9. Determination of association constants carboxylic acids in organic solvents by distribution method.
10. Preparation of colloidal solutions.
11. Verification of F & L adsorption isotherms for acetic acid on activated charcoal.
12. To study the adsorption of iodine on charcoal from alcoholic solution.
13. To study the effects of gelatin solution on the precipitation values.
14. To compare the cleaning powers of two samples of detergents.
15. Any other relevant experiments of interest.

REFERENCES:

1. Findlay's Practical Physical Chemistry, B. P. Levitt, Nabu Press, 2010.
2. Experiments in Physical Chemistry, James and Prichard, 8thEdn, Tata-McGraw Hill, 2008.
3. Experimental Physical Chemistry, Daniels, Nabu Press, 2011.
4. Experimental Physical Chemistry, Das & Behera, Tata McGraw Hill, New Delhi, 1984.
5. Advanced Practical Physical Chemistry, Yadav, 33rdEdn, Krishna Prakashan, 2013.
6. Experiments in Physical Chemistry, J.C.Ghosh, 8thEdn, Tata-Mcgraw Hill, 2008.

PO 589.2- SPECTRAL METHODS OF ANALYSIS

Course Outcome:
Student will be able to:

- Understand theory and application to mass spectrometry, ultraviolet and visible spectroscopy
- Understand infrared spectroscopy, X Ray and
- Gain a basic understanding of nuclear magnetic resonance spectroscopy

UNIT I : ULTRAVIOLET AND INFRARED SPECTROSCOPY **14 Hours**

Beer-Lambert law, instrumentation, molecular vibrations – modes of vibrations

UV absorption spectroscopy: Molar absorptivity, theory of electronic spectra, formation of bands, effect of conjugation with examples; Concept and effect of addition of chromophore and auxochrome. Absorption and intensity shifts- Bathochromic, hypsochromic, hyperchromic and hypochromic shifts. Application of UV spectroscopy in the structural study of organic molecules.

IR spectroscopy: Principle dipole moment, expression to obtain vibrational frequency, force constant, determination of force constant and qualitative relation of force constant and bond energies. Fingerprint region and functional group region. Structural elucidation of simple organic compounds with amino, amide, carbonyl, carboxylic, ester functional groups.

UNIT II : NMR AND MASS SPECTROMETRY **14 Hours**

Shielding and deshielding in NMR, Instrumentation of mass spectrometry

Nuclear magnetic resonance (^{1}H and ^{13}C) Spectroscopy- Chemical shift, factors affecting chemical shift values, spin-spin splitting-predicting the multiplicity of protons. Pascal's triangle. Interpretation of ^{1}H and ^{13}C spectra of simple organic molecules. Basic introduction to 2D NMR.

Mass Spectrometry: Basic principles, ionisation technique MALDI, interpretation of mass spectra, molecular ions, meta-stable ions and isotope ions. Fragmentation processes-representation of fragmentation, basic fragmentation types and rules. Factors influencing fragmentations and reaction pathways. Mc Lafferty rearrangement, retro Diels-Alder fragmentation. Nitrogen rule. Mass spectra of alcohols and aldehydes

UNIT III: DIFFRACTION TECHNIQUES **14 Hours**

X-ray diffraction and electron diffraction basic principles

X-ray diffraction: Bragg condition, Miller indices, Laue method, Bragg method, Debye-Scherrer method, method of x-ray structural analysis, Interpretation of powder patterns, film

method (Weissenberg method). X-ray diffractometers. Systematic absences. Intensities of diffracted X-rays and structural analysis, X-ray scattering by atoms and molecules, Factors affecting X-ray intensities.

Electron Diffraction: Introduction, theory of electron diffraction, Wierl equation and its significance. Structure of surfaces - Low and high energy electron diffraction, TEM, SEM.

REFERENCES:

1. Fundamentals of Molecular Spectroscopy, Banwell & McCash, Tata McGraw Hill, New Delhi, 2007.
2. Spectroscopy, H. Kaur, Pragathi Prakashana, Meerut, 2012.
3. Spectroscopy, Donald L.Pavia, Cengage Learning India Pvt. Ltd., Delhi, 2007.
4. Spectroscopy, B.K.Sharma, Goel Prakashan, Meerut, 2013.
5. A Basic Course in Crystallography, J.A.K Tareen and T.R.N Kutty, University Press, Hyderabad, 2001.
6. Essentials of Crystallography, M.A. Waheb, Narosa Publishing House, New Delhi, 2009.
7. X-ray methods, Clive Whiston, John Wiley & Sons, New York,1987.
8. Organic Spectroscopy, W. Kemp, 3rd Edn, Macmillan, 2011.
9. Spectrometric Identification of Organic Compounds, Silverstein, Bassler & Monnil, 8th Edn, John Wiley & Sons, 2011.
10. Spectroscopy of Organic Compounds, P.S.Kalsi, 6th Edn, New Age Intl., 2004.
11. Molecular Structure and Spectroscopy, G. Aruldhas, 2nd Edn, Prentice Hall, 2009.
12. Spectroscopic Methods in Organic Chemistry, 5th Edn, Williams, TMH, 2004.

THIRD SEMESTER

PH 581.3: ORGANOMETALLIC, BIOINORGANIC AND COORDINATION CHEMISTRY

Course outcomes:

Student will be able to:

- Describe the basic concepts, synthesis, reaction chemistry of organometallic compounds and the structure and bonding patterns.
- Detail the mechanism of different organometallic reactions and catalysis and their application as industrial catalysts.
- Understand the nomenclature, metal-ligand reactions and their mechanism and identify the bonding, structure, and reactivity of selected coordination complexes.
- Understand the role and interaction of Metal ions in biological systems.

UNIT I **14 hours**

Introduction to Organometallic compounds and classification

Classification based on ligands in organometallic compounds, nomenclature, 18-electron rule, counting of electrons in complexes, exception for 18 electron rule. Synthesis, structure and bonding in Li, Be, Mg and Al alkyls. Transition metal complexes with carbenes and carbynes. Synthesis, structure and bonding of transition metal complexes with π–ligands (alkenes, alkynes, dienes, cyclopentadienes, arenes, cycloheptatrienes, COD, COT).

UNIT II **14 hours**

Characteristics of a catalyst, types of catalysis.

Catalysis by organometallic compounds, conditions to be a catalyst, Wilkinson's catalyst, preparation, mechanism of hydrogenation of olefins, Hydroformylation of olefins(oxo process-Cobalt and Rhodium catalysts), mechanism. Isomerization of olefins-mechanism. Oxidation of olefins- Wackers process, steps involved in Wacker's process. Monsanto acetic acid process, Ziegler Natta catalysis-Mechanism. Fisher –Tropsch reaction, Water gas Shift reactions-Mechanism Metal carbene complexes and olefin metathesis: Grubb's and Tebbe's Ragents.

UNIT III **14 hours**

Role of metal ions in biological systems, classification of metal ions and applications of metal ions.

Ion transport across membrane, ionophores, Na^+/K^+ pump, Ca^{++} pump.Transport and storage of dioxygen-Haemoglobin, oxygen uptake, functions of haemoglobin, myoglobin, Physiology of myoglobin and haemoglobin, haemocyanin & hemerythrin.

Metal storage and transport-ferritin, transferrin and ceruloplasmin.

Electron transfer proteins-cytochromes- cytochrome c, iron sulphur proteins

Nitrogen fixation, bacterial nitrogenase enzyme.

Unit IV **14 hours**

Types of substitution reactions, S_N1 and S_N2 reactions and their mechanisms.

Reaction mechanisms in transition metal complexes: Energy profile of a reaction, inert and labile complexes, kinetics of octahedral substitution and mechanistic aspects. Acid hydrolysis, Factors affecting acid hydrolysis, mechanism of acid hydrolysis, base hydrolysis, conjugate base mechanism. Substitution reactions in square planar complexes, trans effect, theories of trans effect, mechanism of substitution. Electron transfer reactions- inner sphere and outer sphere reactions, complimentary and non complimentary reactions.

REFERENCES

1. Organometallic Chemistry, R.C Mehrotra and A.Singh, John Wiley, 1991.
2. The Organometallic Chemistry of the Transition Metals, R.H Crabtree, John Wiley, 2014.
3. Principles and Application of Organotransition Metal Chemistry, Akio Yamamoto, John Wiley, 1986.
4. An Introduction to Organometallic Chemistry, A.W Parkins and R.C Poller, Palgrave, 1986.
5. Organo transition Metal Chemistry, S.G Davies, Macmillan, 1987.
6. Inorganic Chemistry, J.E.Huheey, E.A Keiter, 4thEdn, Pearson, 2006.
7. Principles of Inorganic Chemistry, Puri, Sharma and Kalia, 33rdEdn, Vishal Pubs, 2016.
8. Organo metallic, J L Jain, ebook.
9. Bioorganic, bioinorganic and supramolecular chemistry, P.S.Kalsi and J.P.Kalsi, 4th Edn., New Age International, 2007.
10. Bioinorganic Chemistry, Asim K.Das, 2nd Edn.,CBS Publishers & Distributors, New Delhi, 2012.
11. Principles of Bioinorganic Chemistry, Stephen J. Lippard, Jeremy Mark Berg, University Science Books, 1994.
12. Basic Organometallic Chemistry: Concepts, Syntheses and Applications By A J Elias B D Gupta, Universities Press, 2013.

PH 582.3: ELECTROCHEMISTRY AND THERMO-ANALYTICAL METHODS

Course outcomes:
Student will be able to:

- Detail the structure of electrode-electrolyte interface with various models such as Helmholtz - Perrin, Gouy - Chapman and Stern model of electrical double layers.
- Describe the physical principles of Photo electrochemistry and its classification.
- Understand the basic principles of corrosion science.
- Describe the methods of corrosion protection and explain the principles of corrosion protection.

UNIT I **14 hours**

Introduction to electrode-electrolyte interface; conductors, semiconductors and insulators; structural treatment of ion-dipole interaction.
Electrical double layer: Thermodynamics of electrified interface,Lipmann equation. structure of electrified interface: Helmholtz - Perrin, Guoy-Chapman and Stern models. Competition between water and organic molecules at the electrified interface.Theory of double layer at semiconductor-electrolyte solution interface.
Ion-solvent Interaction: Ion-Solvation-Introduction, evidence for solvation, Structural aspects of ion-solvent interaction -Born model and its limitations, structural treatment and ion-quadruple models. Spectroscopic and Thermo chemical approach to ion-solvent interaction.Solvation number– Introduction, methods of determination.

UNIT II: **14 hours**

Reference electrodes- calomel, silver/silver chloride and hydrogen electrodes

Fundamentals of potentiometry. Indicator and ion-selective electrodes. Electrodes of first, second, third kind and redox type. Membrane electrodes. Glass electrode for pH measurement, glass electrodes for cations other than protons. Liquid membrane electrodes, solid state ion selective detectors and biochemical electrodes. Potentiometric end point detection. Applications of potentiometry.

Voltammetric Techniques: Polarization: Sources, overvoltage, concentration polarization, mechanism of mass transport Theory of classical polarography, polarograhic measurements, polarograms, polarographic currents. Current and concentration relationship. DC polarography-IlKovic equation, half wave potential, applications of polarography, Pulse Polarographic techniques, Cyclic voltammetry.
Stripping Analysis: Principle, methodology, electrodes and cell design, Applications.
Amperometry: Principle, titrations, advantages and limitations. Biamperometric titrations.
Coulometry: Principle, constant current and controlled potential coulometry. Applications of coulometric titrations

UNIT III **14 hours**

Semiconductor electrode types and stability

Photoelectrochemistry: Introduction, photogalvanic cells, photoelectrochemical cells.

Electrochemical Energy System: Introduction to electrochemical energy systems and solar energy system, Electricity storage-Importance, storage density, Primary battery (Laclanche-dry cell and Alkaline cell). Secondary battery (acid and alkaline).Reserve batteries. Fuel cells (H2-O2, methanol, bio-cells).

Industrial Electrochemistry : Fundamentals, electro- organic synthesis (Kolbes synthesis, adiponitrile, oxidation & reduction of hydrocarbons, reduction of nitro-compounds). Electro-inorganic synthesis of fluorine, chlorates & ozone

UNIT IV **14 hours**

Effect of temperature on solids, liquids, gases, and on hydrated organic and inorganic compounds.

Corrosion: Introduction, Types of corrosion-galvanic, localized, atmospheric and microbial, methods of prevention-design improvement, anodic and cathodic protection, use of inhibitors, Passivation, Galvanic series, Thermodynamic & kinetics of corrosion. Factors affecting corrosion rate.

Thermoanalytical Techniques: Introduction, thermogravimetric analysis(TGA), types of thermogravimetric analysis, principle and methods. Automatic thermogravimetric analysis, instrumentation, types of recording thermobalances, sample holders, factors affecting results and applications. Differential thermal analysis (DTA)-principle of working, theory and instrumentation. Simultaneous DTA-TGA curves, factors affecting results and applications. Differential scanning calorimetry(DSC)- principles, instrumentation and applications.

Thermometric titration: Introduction, apparatus and applications (Acid-base, precipitation, complexation, redox and non-aqueous titrations)

REFERENCES:

1. Modern Electrochemistry, Bockris and Reddy, 2ndEdn, Springer, 2008.
2. Chemical and Electrochemical Energy Systems, Narayan &Viswanathan, 1stEdn, Universities Press,1998.
3. Biosensors-Theory and Applications, Donald G.Buerk, 1stEdn, CRC Press, 1995.
4. Fundamentals of Analytical Chemistry, S.A. Skoog, West & Holler, 9thEdn, Cengage Learning, 2014.
5. Instrumental Methods of Chemical Analysis, B.K. Sharma, 29thEdn, Krishna Prakashan Media, 2014.
6. Principles of Electroanalytical Methods, T.Riley and C.Tomlinson, Wiley India, 2011.
7. Principles of Instrumental Analysis, D.A. Skoog, 6thEdn, Cengage, 2014.
8. Quantitative Analysis, R.A. Day and A. L. Underwood, 6thEdn, PHI Learning Pvt Ltd, 2008.
9. Vogel's Text book of Quantitative Inorganic Analysis, Bessett, Denney, Jeffery & Mendham, 6thEdn, Pearson India, 2009.
10. Electro-Analytical Techniques, V. B. Pathania, 1stEdn, Cumpus Book International, 2004.
11. Electrochemical methods- fundamentals and applications, Allen Bard & Larry Faulkner, 2ndEdn, Wiley India Pvt Ltd, 2006.
12. Instrumental methods of Chemical Analysis-Gurdeep R Chatwal, 5thEdn, Himalaya Publishing House, 2007

PS 583.3: MOLECULAR SPECTROSCOPY

Course outcomes:

Student will be able to:

- Gather knowledge about various spectroscopic techniques such as IR, NMR UV and Mass spectroscopy analysis.
- Understand theory and application to mass spectrometry, ultraviolet and visible spectroscopy, infrared spectroscopy, nuclear magnetic resonance spectroscopy.
- Apply NMR, IR, MS, UV-Vis spectroscopic techniques in solving structure of organic molecules.

UNIT - I **14 hours**

Theory of NMR, nuclear spin and magnetic spin chemical shift and its measurements

Nuclear Magnetic Resonance Spectroscopy: Magnetic properties of nuclei, NMR spectrometer, FT-NMR and its advantages. Solvents used, factors affecting chemical shift. Integration of NMR signals, spin-spin coupling, coupling constant. Shielding and deshielding. Chemical shift assignment of major functional groups, Classification (ABX, AMX, ABC, A_2B_2 etc.), spin decoupling; effects of chemical exchange, fluxional molecules, Hindered rotation through NMR spectrum, Karplus relationships (Karplus curve–variation of coupling constant with dihedral angle), double resonance techniques, NMR shift reagents, solvent effects and Nuclear Overhauser Effect (NOE). High resolution ^{1}H NMR spectroscopy. Use of NMR in Medical diagnostics.

Introduction to 2 D techniques: COSY

NMR studies of nuclei other than proton: ^{13}C chemical shift and factors affecting the chemical shift, Coupling constants. Decoupling-Noise decoupling and broad band decoupling. Off-resonance proton decoupling-some representative examples.

UNIT - II: **14 hours**

Factors affecting chemical shift and coupling constants

Beer-Lambert's law, Auxochromes and Chromophores

UV/Electronic Spectroscopy: Woodward, Woodward–Fieser rules. UV absorption of aromatic compounds - effect of substituents and solvent effects. Emperical rules to calculate λmax. Spectrophotometric titrations and simultaneous determinations.

Mass Spectrometry: Basic principles, Instrumentation - Mass spectrometer, interpretation of mass spectra, resolution, molecular ions, meta-stable ions and isotope ions. Fragmentation processes-representation of fragmentation. Factors influencing fragmentations and reaction pathways. McLafferty rearrangement. Fragmentations(fragmentation of organic compounds with respect to their structure determination) associated with functional groups- alkanes, alkenes, cycloalkanes, aromatic hydrocarbons, halides, alcohols, phenols, ethers, aldehydes, ketones, carboxylic acids, esters, amides, amines and nitrogen heterocycles. Ion analysis, ion abundance, retro Diels-Alder fragmentation. Nitrogen rule.

UNIT –III **14 hours**

Types of molecules showing vibrational spectra, types of molecular vibrations (i.e., IR active & IR inactive)

Application of infrared spectroscopy in the structural study-identity by fingerprinting and identification of functional groups. Characteristic vibrational frequencies of common functional groups (alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines).study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, etc.). Factors affecting band positions and intensities such as effect of hydrogen bonding, phase and solvent on vibrational frequencies, overtones, combination bands and Fermi resonance. NIR and FIR spectroscopy.

Structural Elucidation

Determining the structure of organic compounds from the combination of spectra. Presence of fragments from the mass spectrum, relative number of protons in different environments from the ^{1}H NMR spectrum, number of carbons in different environments from ^{13}C spectrum, the presence or absence of functional groups from IR spectrum and examining the UV spectrum for evidence of conjugation, aromatic rings etc.

REFERENCES:

1. Fundamentals of Molecular Spectroscopy, Banwell & McCash, 4thEdn, Tata McGraw Hill, 2004
2. Organic Spectroscopy, W.Kemp, 3rdEdn, Mac, 2011.
3. Spectrometric Identification of Organic Compounds, Silverstein, Bassler & Monnil, 8thEdn, John Wiley & Sons, 2011.
4. Applications of Absorption Spectroscopy of Organic Compounds, Dyer, 1stEdn, PHI Learning, 2011.
5. Spectroscopy of Organic Compounds, P.S.Kalsi, 6thEdn, New Age Intl, 2004.
6. Molecular Structure and Spectroscopy, G.Aruldhas, 2ndEdn, Prentice Hall, 2009.
7. NMR Spectroscopy in Inorganic Chemistry, J. A. Iggo, Oxford University Press, 2000.
8. Spectroscopic Methods in Organic Chemistry, 5thEdn, Williams, TMH, 2004.
9. Carbon-13 NMR Spectroscopy, E. Breitmer and W. Voeller, 3rdEdn, VCH, Weinheim, 1987
10. Two Dimensional NMR Spectroscopy, W. R. Croasmum and R. M. K. Carlson,2ndEdn, John Wiley, New York, 2000.
11. Organic Structures from Spectra, L D field, 5thEdn, 2013.

PS 584.3 :MEDICINAL CHEMISTRY

Course outcomes:
Student will be able to:

- Explain the mechanism of drug action and drug designing.
- Understand the classification, structure and mechanism of drugs action.
- Develop an understanding on various CNS depressants

UNIT I : **14 hours**

Introduction to drugs, classification and nomenclature of drugs

Drugs : Theories of drug action. Drug design, analogues and pro drugs. Factors governing drug design, rational approach to drug design, tailoring of drugs, Physico-Chemical factors and Biologocal activities. Factors governing ability of drugs.

General Anaesthetics: Introduction and classification. Synthesis of Halothane, Methoxyfluorane and Methohexital sodium.Thiamyl sodium, mode of action.

Local Anaesthetics: Introduction and classification. Synthesis of benzocaine, butamben, Procaine hydrochloride, tetracaine hydrochloride, butacaine sulphate, α-eucaine, Benamine hydrochloride, Lignocaine, Prilocaine and Mepivacaine. Mode of action of benzocaine, butacaine sulphate, Mepivacaine, Procaine hydrochloride and Prilocaine

UNIT II :14 hours

Analgesics, Narcotics and non-narcotics

Antibiotics: Mechanism of action of following antibiotics, Pencillin-Strereochemistry, Synthesis of Pencillin-G, Chemical degradation and bacterial resistance.

Cephalosporians- Nomenclature, degradation and B-Lactumase resistance.Tetracyclines, Streptomycin and Chloramphenicon-SAR studies.

Analgesics and anti inflammatory agents: Narcotic and non-narcotic agents- Introduction and mechanism of action. Synthesis of Ibuprofen, Acetaminophen and Phenyl butazone.

Antiarrythmic agents: Introduction, mechanism of action and synthesis of verapamil.

Antihypertensive agents: Introduction, Mechanism of action, Synthesis of Clonidine and Hydralazine derivatives.

Hypoglycemic Agents : Introduction, Mechanism of action, synthesis of Tolbutamide and Tolazamide.

Anti-Amoebic agents: Introduction, Classification, Mechanism of action, synthesis of metronidazole, Iodoquinol and dimercaprol.

UNIT III: **14 hours**

Introduction and classification of CNS depressants

CNS depressants: Sedative and hypnotic agents: Synthesis of Barbitone, Methylphenobarbital, Butobarbitone, Chloradiazepoxide, Diazepam, Phenobarbital.

AntiConvulsants : Synthesis of Phenytoin sodium, Trimethadion, Carbamazepine.

CNS Stimulants : Introduction and classification. Synthesis and mechanism of action of caffeine, Nikethamide, Phetermine, Methylphenidate.

Anti Histaminic Agents: Mechanism of action, synthesis of Diphenhydramine hydrochloride, Pyrilamine, Pheniramine.

Anti Malarials : Etiology of Malaria, mechanism of action and SAR studies of Quinolines antimalarials. Synthesis of Chloroquin, Primaquin and Quinacrine.

REFERENCES :

1. Medicinal Chemistry, Ashutosh Kar, 5thEdn, New Age, 2010.
2. Medicinal and Pharmaceutical Chemistry - H Singh and V K Kapor, Vallabh Praskashan, New Delhi,1996.
3. Burger's Medicinal Chemistry Series, Alfred Burger, 3rdEdn, John Wiley & Sons, 1970.
4. Medicinal Chemistry of anti Cancer drugs - Carmen Avendalo and J C Menedez, 1stEdn, Elsevier Science, 2008.
5. General Analgetics - Daniel Ladnicer, John Wiley & sons Inc, 1982.
6. The Organic Chemistry of Drug Synthesis, Daniel Ladnicer, 7thEdn, Wiley Blackwell, 2007.
7. Medicinal Chemistry, A Molecular and Biochemical Approach, Thomas Nogrady and Donald F Weaver, 3rdEdn, Oxford University Press, 2005.

PS 585.3P: COMPUTERS FOR CHEMISTS - PRACTICALS

Course Outcome:

Student will be able to:

- Understand about the different operating systems and software's
- Get a training on using subject specific software's.
- Get hands-on experience to use the relevant software's

UNIT-I **14 hours**

Overview of the computer system, parts of the computer system, physical components. How to operate a PC,MS-Word and MS-Power Point basics.

Introduction to computers and computing: Basic structure and functioning of computers with a PC as an illustrative example. Memory, I/O devices. Secondary storage. . Data processing, principles of programming. Algorithms and flow charts

Operating Systems & Word Processing:

Basic Idea of DOS, WINDOWS, UNIX & Android;

Working with MS-Word: Formatting text & documents, sorting & tables, Introduction to mail merge, Reference Writing.

MS-Power Point: Working with graphics and creating presentation the easy way, show time, sound effects and animation effects.

UNIT-II **14 hours**

Concept of spreadsheets, Functions and Formulas of MS Excel, LAN and World Wide Web, Application software installation.

Use of Computer Programmes: Software packages such as MSEXCEL, ORIGIN, CHEM SKETCH,CHEMDRAW, BIOVIADRAW etc. and special emphasis on calculations and chart formations. Problems will be taken preferably from physical chemistry for plotting first and second derivative curves, linear plots etc. Writing the structures of inorganic and organic molecules, writing chemical equations, determining molecular parameters such as bond lengths, bond angles, dihedral angles etc.

Internet- Application of Internet for Chemistry with search engines, various types of files like PDF, JPG, RTF and Bitmap. Scanning, OMR, Web camera.

COMPUTER PRACTICALS -

MS WORD/POWERPOINT

1. Page Setup, Save, Open, Close files, Fonts size, Borders & Shading, Alignment, Superscript, Subscript, etc.
2. Changing Indents, formatting paragraph options.
3. Columns, Inserting Symbols, Date, Time, Applying Bullets and Numbering, Page Break and Page Numbers, Word Art
4. Inserting picture, Drawing objects, Numbering and Spell Check, Line Spacing, Drop Cap.
5. Table, Merge Cells, Text Direction, and Paragraph Space before and after.

6. Mail Merge for 5 addresses.
7. Inserting Footnote, Creating and applying styles, Change Case Find and Replace and Autocorrect.
8. Reference Writing and reviewing a document.
9. Creating presentation with show time, sound effects and animation effects for any given topic**.**

MS EXCEL/ORIGIN: Plots and Calculations for physical chemistry problems.

1. Potentiometric determination of redox potentials.
2. Potentiometric determination of dissociation constants of weak acids.
3. Conductometric titrations of displacement and precipitation reactions.
4. Potentiometric titration of halides in mixtures.
5. Determination of pH of buffer solutions with a pH meter & evaluation of pKa of acids.
6. Determination of maximum wavelength of the sample from transmittance data.
7. Calculate the various statistical information.
8. Energy of activation from rate constant.
9. Beer-lamberts law and molar extensive coefficient.
10. Average molecular weight and molecular weight distribution of the polymer sample.

CHEMSKETCH/CHEMDRAW/BIOVIADRAW: structures of inorganic and organic molecules

1. Structures and diagrams (Ligands, Indicators)
2. Canizzarro reaction
3. Benzil-Benzilic acid Rearrangement
4. Preparation of adipic acid from cyclohexanol.
5. Preparation of p-nitrobenzoic acid.
6. Vilsmeir-Haack reaction
7. Bischler-Napieralski reaction
8. Fischer indole synthesis

REFERENCES:

1. Introduction to Computers,Peter Norton, 6thEdn,Tata McGraw Hill, New Delhi, 2008.
2. Computers and their applications to Chemistry, Ramesh Kumari, 2ndEdn, Narosa Publishing House, 2011.
3. Theory and Problems of Programming with Basic, Goldberg, 1stEdn, Mcgraw Hill, NY, 2002.
4. Computer programming in Fortran IV,V, Rajaraman, 4thEdn, Prentice Hall of India, 2009.
5. Computers in Chemistry, K. V. Raman, 1stEdn, TMH, 2004.
6. BIOVIA Draw document Retrieved from http://accelrys.com/products/pdf/biovia-draw-ds.pdf
7. CambridgeSoft User's Guide version 9.0.1, 2004, Retrieved from http://www.cambridgesoft.com/support/DesktopSupport/Documentation/Manuals/files/chemdraw_9_english.pdf

PS 586.3P: INORGANIC CHEMISTRY PRACTICALS – III

Course outcomes:

Student will be able to:

- Estimate binary mixtures of metallic ions in solution
- Detect presence of certain type of ions in water.

A. Any five of the following experiments are to be carried out:

1. Analysis of brass – Cu gravimetrically using ∝-Benzoin oxime and Zinc complexometrically.
2. Analysis Cu-Ni alloy.
3. Analysis of Stainless Steel – Insoluble residue by gravimetry, Ni gravimetrically Using DMG, Fe volumetrically using Ce(IV) & Cr(III) volumetrically by persulphate oxidation.
4. Analysis of Type metal –Sn gravimetrically, Pb electrogravimetrically and Sb titrimetrically using $KBrO_3$
5. Quantitative analysis of the constituents & mixtures containing the following radicals
   (i) Cu(II) + Fe(II) - Cu gravimetrically as CuSCN and Fe using Ce(IV).
   (ii) Fe(II) + Ni(II) – Fe gravimetrically as Fe_2O_3 and Ni using EDTA.
   (iii) Fe(III) + Ca(II) - Fe gravimetrically as Fe_2O_3 and Ca using EDTA.
   (iv) Cr(III) + Fe(III) – Using EDTA by Kinetic masking method.
6. Analysis of chalcopyrites, magnetite and ilmenite.
7. Ion-exchange chromatography: Separation and determination of Mg^{2+}/Zn^{2+}, Zn^{2+}/Cd^{2+}&Cl^-/ Br^-.

B. Any five of the following experiments are to be carried out:

8. Determination of COD of a water sample
9. Determination of Phosphorus.
10. Determination of dissolved oxygen (DO) by Winkler's method
11. Determination of nitrite in water samples .
12. Analysis of heavy metals in waste water, sea water (Pb, Hg etc. By spectrophotometry)
13. Determination of available K in soil,
14. Nephelometric determination of sulphate/phosphate.
15. Determination of alkalinity of water samples
16. Determination of fluoride in toothpaste by spectrophotometry and ion selective electrode
17. Determination of phosphates in detergents
18. Spectrophotometric determination of sulphur and phosphorus present in soil.

REFERENCES:

1. APHA, AWWA and WPCF: Standard Method for the Examination of water and Waste Water (Washington DC), 22nd Edn, Amer Public Health Assn, 2012.
2. Environmental Chemistry, I.Williams, Wiley, 2001
3. Comprehensive Analytical Chemistry, Lobinski and Marczenko, Elsevier Science, 1996.

PS 587.3P ORGANIC CHEMISTRY PRACTICALS – III

Course outcomes:
Student will be able to:

- Separate and perform systematic qualitative analysis of binary mixtures of organic compounds containing both mono and bifunctional groups and preparation of suitable derivatives.

Quantitative determination of sugars, amino acids, phenols, carboxylic acids, amides, esters, aldehydes, ketones, urea by various methods. Determinations of acid and ester and acid and amide in mixtures of two.
Determination of functional groups like hydroxyl, vic-hydroxyl, enol, amino, amide.

REFERENCES :

1.Practical Organic Chemistry, F .G. Mann and B. C. Saunders, 4thEdn, Pearson India, 2009.
2. Practical Organic Chemistry, A. I. Vogel, 5thEdn, Pearson India, 2005.
3. Vogel's Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis, B. S. Furniss et al, 2ndEdn, Pearson India, 2010.

PS 588.3P : PHYSICAL CHEMISTRY PRACTICALS – III

Course outcomes:
Student will be able to:

- Carry out experiments related to chemical kinetics, Polarimetry, Conductometry and Potentiometry

A. Electrochemistry:

a. Conductometry (At least Three experiments to be carried out)

1. Determination of hydrolysis constants (aniline hydrochloride etc.).
2. Titration of a mixture of acetic acid, monochloro and trichloroacetic acids with NaOH.
3. Determination of concentrations/amounts of sulphuric acid, acetic acid and copper sulphate by conductometric titration with sodium hydroxide.
4. Determination of oxalic acid by conductometric titration with sodium hydroxide.
5. Measurements of the conductance of a weak acid, AcOH and of the strong electrolytes NaOAc, HCl and NaCl and to calculate the ionisation constant of the acid.
6. Determination of pH and pK_a of a given weak acid at various dilutions.
7. Conductometric titration of the mixture of HCl and NH_4Cl.
8. Determination of activity coefficient of Zinc ions in 0.002M $ZnSO_4$.
9. Any other experiments of interest

b. Potentiometry (At least Three experiments are to be carried out)

1. Determination of pK_a values of maleic acid/malonic and phosphoric acid by potentiometric titration with sodium hydroxide using glass electrode.
2. Determination of acidic and basic dissociation constants and isoelectric point an amino acid.
3. Determination of the potential of an electrochemical cell and mean ionic activity coefficient .
4. pH titration of (a) HCl versus NaOH, (b) $CuSO_4$ versus NaOH and (c) AcOH versus NaOH and (d) lead nitrate versus potassium chromate.
5. Determination of pK_a values of functional groups in amino acids using a pH meter.
6. Study of potential-pH diagrams.
7. Determination of activity coefficient of an electrolyte at different molalities.
8. Verification of Tafel equation of hydrogen evolution reaction.
9. Determination of pKa values of mono, di and tri-acid base.

B. Photochemistry (Any Two experiments are to be carried out**)**

1. Irradiation of a reaction mixture and calculation of the quantum yield.
2. Determination of the quantum yield of chloride in the photohydrolysis of aqueous solution of monochloroacetic acid
3. Photochemical study of decomposition of hydrogen peroxide.
4. Photochemical study of Bleaching of dyes.
5. Photochemical reaction between threonine and ferrous sulphate.

C. Voltammetry & Polarography*(Any Three experiments are to be carried out)*

1. Determination of the half-wave potential of Cd(II), Cu(II)& Zn(II) ions in 0.1M solutions.
2. Determination of metal ions individually and in mixtures,
3. Determination of the formula and the stability constant of a lead oxalate.
4. Study of the polarogram of supporting electrolyte with and without dissolved oxygen,
5. Determination of Huckel β value of aromatic hydrocarbon reduction at dropping mercury electrode.

REFERENCES

1. Findlay's Practical Physical Chemistry, B. P. Levitt, Plenum Publishing Corporation, 1973.
2. Experimental Physical Chemistry, Daniels et al, 1st Edn, CBS Publisher, 2006.
3. Experimental Physical Chemistry, Das &Behera, Mcgraw-Hill Education ,1984.
4. Advanced Practical Physical Chemistry, J. B. Yadav, 33rd Edn, KRISHNA Prakashan Media (P) Ltd, 2013.
5. Experiments in Physical Chemistry, J.C.Ghosh,8th Edn, Tata McGraw-Hill Education, 2008.

PO589.3 - BIO-INORGANIC CHEMISTRY, GREEN CHEMISTRY AND ENVIRONMENTAL CHEMISTRY

Course outcomes:

Student will be able to:

- Understand the role and interaction of Metal ions in biological systems.
- Understand the principle and importance of green chemistry.
- Identify environmental problems related to pollution , identify and utilize eco-friendly methods to protect it, understand and apply green chemical methods solve the problems related to environmental pollution.

UNIT I : BIO-INORGANIC CHEMISTRY 14 Hours

Na^+/K^+ pump, physiology of haemoglobin

Role of metal ions in biological systems, classification of metal ions and applications of metal ions. Ion transport across membrane, ionophores, Ca^{++} pump.Transport and storage of dioxygen-Haemoglobin, oxygen uptake, functions of haemoglobin, myoglobin, Physiology of myoglobin, haemocyanin & hemerythrin.

Metal storage and transport-ferritin, transferrin and ceruloplasmin.

Electron transfer proteins-cytochromes- cytochrome c, iron sulphur proteins

Nitrogen fixation, bacterial nitrogenase enzyme.

UNIT II : GREEN CHEMISTRY 14 Hours

Introduction, Basic principles of green chemistry

Atom economy, Tools of Green Chemistry. Zero Technology. Solvent free reactions-Utility of solvent free conditions, controlling solvent free reactions. Solvent free techniques-Reaction on solid mineral supports, Solid-Liquid Phase Transfer Catalysis (PTC), Organic synthesis under Microwaves. Comparison between green and conventional methods of synthesis with suitable examples.

UNIT III : ENVIRONMENTAL CHEMISTRY 14 Hours

Classification and properties of air pollutants; Types of water pollutions, their sources and effects

Air Pollution Analysis and Control Methods : Chemical reactions in the atmosphere, photochemical smog. Analysis of air pollutants like SO_2 , NOx , CO. Control of gaseous emissions. SO_2 –desulphurisation of fuels and flue gases

Water Pollution and Treatment: Causes and prevention.

Water Treatment : Drinking water, desalination - (Reverse osmosis, FD, Electro Dialysis), sewage treatment, Industrial waste water treatment – (sugar, textile, leather)

Environmental Toxicology : Toxic chemicals in the environment, impact of toxic chemicals on enzymes, biochemical effects of arsenic, cadmium, mercury, lead. Carcinogens.
Brief introduction on the role of nanotechnology in environmental studies.

REFERENCES

1. Bioorganic, bioinorganic and supramolecular chemistry, P.S.Kalsi and J.P.Kalsi, 4th Edn., New Age International, 2007.
2. Bioinorganic Chemistry, Asim K.Das, 2nd Edn., CBS *Publishers* & Distributors, New Delhi, 2012.
3. Principles of Bioinorganic Chemistry, Stephen J. Lippard, Jeremy Mark Berg, University Science Books, 1994
4. Environmental Chemistry – S.E. Manahan, Lewis Pub., 4th Edn., Columbia,1990.
5. Air Pollution – B.G. Liptak, Lewis Publishers, 2000.
6. Water Pollution – B.G. Liptak, Lewis Publishers, 2000.
7. Environmental Chemistry – A.K. De, Prentice Hall of India, 1987
8. Environmental Pollution Control and Engineering – C.S.Rao, Wiley-Eastern, New Delhi,1991
9. Standard Methods for Examination of Waste Water – Ed. Greenberg, Connors and Jenkins, 15th Edn., APHA,1981.
10. Instrumental Analysis for Water Pollution Control – M.Nancy, Ann Arbor, Michigan, 1971
11. Environmental Chemistry, Balram Pani, I K Intl Publishing House, 2007
12. New Trends in Green Chemistry, V.K. Ahluwalia, M. Kidwai, Anamaya Publishers, 2004.

SEMESTER IV

PH 581.4: ORGANIC SYNTHETIC METHODS

Course outcomes:

Student will be able to:

- Understand and apply the various reagents in organic synthesis and design organic synthetic reactions.
- Describe the applications of oxidation and reduction techniques in organic synthesis.
- Prefer suitable reagent for important reactions/building appropriate bonds.
- Understand the principles and applications of protecting groups in chemistry.

UNIT I: **14 Hours**

Introduction and different types of reductions

Reduction Reactions: Catalytic hydrogenation: Catalysts and solvents employed, reduction o functional groups, mechanisms and stereochemistry of catalytic hydrogenations, Hydrogenolysis an homogenous catalytic hydrogenation. **Metal hydride reduction:** Reduction with LiAlH4, NaBH4 Stereochemistry of reduction and other functional groups, Functional group transformation durin reduction. Reduction with diborane and related reactions. Reduction in Biological systems-NADH FAD.

Dissolving metal reductions: Mechanism of reduction of conjugated systems and carbony compounds. Bimolecular reduction of esters, Birch reduction, Wolf-Kishner reduction, Clemmense reduction, reduction with derivatives of hydrazine. Reduction with arene sulphonyl derivatives o hydrazine, Reaction with di-imide and related compounds.

UNIT II **14 Hours**

Introduction to oxidation, different types of oxidative processes.

Oxidation Reactions: Mechanism of oxidation reaction with chromium and manganese salts peracids, peresters, periodic acids, Lead tetraacetate, ozone, osmium tetroxide , Selenium dioxid and their synthetic importance in functional group transformation.

Molecular rearrangements: Mechanism of Wagner-Meerwein, Dienone-Phenol, Pinacol Pinacolone, Demaynov, Benzil-Benzilic acid, Fries, Wolff, Favorskii, Neber, Benzidine, Baeyer Villiger, Beckmann, Lossen, Curtius, Schmidt, Stevens, Shapiro, Baker-Venkatraman and Amadoı rearrangement.

UNIT III **14 Hours**

Introduction of C-C and C=C into the molecules using various reactions,

Synthetic Designs: Carbon skeleton framework, classification of carbon-carbon single and doubl bonds forming reactions and their use in carbon skeleton ring formation. ring forming and rin cleaving reactions, use of Thorpe condensation, Carbene insertion reaction, Friedel-Crafts reactior 1,3-dipolar addition and ene reaction in ring formation, Oxidative cleavage of rings and Retro-Diel' Alder reactions.

Planning of Organic synthesis: Selection of starting materials and key intermediates during th synthesis. Synthesis of Cubane. Use of Robinson annulations, Dickmann cyclization, Arndt -Eiste homologation and Diel's Alder reaction in organic synthesis. Suzuki coupling, Heck reactio Negeshi coupling, Sonagashira reaction.

Functionality: Synthesis of 6/7-methoxy tetralones, biotin and Pencillin-V with special reference t the introduction of functional groups. Stereochemical consideration and stereo selectivity durin organic synthesis.

UNIT IV **14 Hours**

Interconversion of functional groups and principle of protection of functional groups

General introduction to disconnection approach: Basic principles and technologies used i disconnection approach. Synthons and Synthetic equivalents. Interconversion of functional groups One group C-X and two group C-X disconnections. Protecting groups: Principle of protection o hydroxyl, amino, carboxylic acid and carbonyl groups.C-C one and C-C two group disconnectio Multistep synthesis of benzocaine, Phenacitin, 2,4-dichloroacetic acid,4-Hydroxy-4-methy pentanone, 2,5-dimethyl-3- hexanone, 2-methyl-6-methoxy indole 3-acetic acid. 6-methylquinoline & 1-phenyl-4-p-methoxyphenyl-1,3-butadiene, Limonene, Danishefsky's pentalenolactone Benziodarone, nitrofurazone, Warfarin and Juvabione.

REFERENCES:

1. Modern Organic Reactions, G. Whitmore, 1st Edn, Ivy Publishing House, 2008.

2. Organic Reaction Mechanisms, Fourth Edition, V.K. Ahluwalia and Rakesh Kumar Parashar

3. March's Advanced Organic Chemistry, Reactions, Mechanisms and Structure, Michael B. Smit and Jerry March, 6th Edition, 2013

4. Organic Synthesis - The Disconnection Approach, Stuart Warren, 2nd Edn, Wiley, 2010

5. Advanced Organic Chemistry, Carrey & Sundberg, 5th Edn, Springer, 2007.

6. Modern Methods of Organic Synthesis, N. Carruthers, 4th Edn, Cambridge University, 2004.

7. Organic chemistry, Claydon, 2nd Edn, Oxford Univ Press, 2012.

8. Modern Organic Chemistry, M K Jain & S C Sharma, 4th Edn, Vishal Publishing House, 2011

PH 582.4 : RADIATION AND PHOTOCHEMISTRY

Course outcomes:
Student will be able to:

- Demonstrate a systematic understanding of the key aspects of nuclear chemistry and their analytical applications
- Acquire knowledge of nucleus, nuclear reaction, radioactive techniques and application of radioisotopes.
- Describe the methods of measurements and kinetics of photochemical reactions
- Discuss the principle of absorption and emission of radiation and explain the mechanism of Jablonski diagram

UNIT - I: **14 hours**

Definition, Natural and artificial radioactivity, characteristics of $\propto$, β and γ rays

Nuclear structure and stability: Nuclear properties - nuclear forces, mass defect and binding energy. Nuclear stability-Liquid drop, shell and collective models.

Radioactivity and Nuclear Decay: Decay modes of natural and artificial nuclides- Determination of half-life, growth kinetics. Conditions of equilibrium.

Radiation Detection and Measurement: Experimental techniques in the assay of radioactive isotopes. Radiation Detectors-ionization chambers, proportional and Geiger-Muller, scintillation and semiconductor radiation detectors (NaI-Tl and Ge(Li), HPGe solid state detectors). Liquid scintillators and multichannel analyzers.

Nuclear Reactions, Energy and Nuclear Power reactors: Nuclear fission and fusion. Types of nuclear power reactors, basic features and components of a nuclear power reactor. An introduction to breeder reactors.

UNIT – II **14 hours**

Health and Safety Aspects*: Biological effects of radiation, Hazards in radiochemical work. Radiation protection, permissible exposure doses. Radioactive waste management.*

Radioisotopes: Definition of curie and related calculations. Production of radioisotopes and labelled compounds by bombardment. Radiochemical separation techniques- carriers, solvent extraction and ion-exchange methods. Szilard-Chalmer process. Physico-chemical and analytical applications-isotope dilution method, activation analysis, PGNAA, neutron absorptiometry, radioimmune assay, radiometric titration, determination of the age of the aquatic life and age of the minerals and C-14 dating. Medical, agricultural and industrial applications of isotopes.

Radiation Chemistry: Difference between radiation and photochemistry. Radiation sources, units (LET, Rad, Roentgen and G-value), radiation dose and radiation chemical yield. Chemical Dosimetry-Fricke and ceric sulphate dosimeters. Radiation chemistry of water. A brief introduction to radiolysis of gases, liquids and solids. Techniques for study of transient species- Pulse radiolysis.

UNIT- III: **14 hours**

Photochemical reactions, Definition of Quantum yield

Introduction to photochemistry, difference between thermal and photochemical processes., determinations of Quantum yield, experimental methods in photochemistry, Actinometry. Electronic energy states of atoms and molecules -rules for transition between two energy states. Life time of excited electronic states, Frank- Condon principle. Absorption and emission spectra-effect of solute solvent interactions on electronic spectra-spectral shifts. Physicochemical properties of electronically excited molecules-excited state dipole moments, acidity constants. Study of excited states by flash photolysis and laser beam experiments.

UNIT -IV: **14 hours**

Fluorimetric and phosphorimetric applications, Applications of photochemistry in organic synthesis and atmospheric chemistry.

Photophysical pathways: Jablonski diagram, radiative and Radiationless transitions and selection rules. Molecular Luminescence- Flourimetry and phosphorimetry- theory, factors affecting flourescence and phosphorescence. Relationship between intensity of fluorescence and concentration, instrumentation- basic differences in the measurement of fluorescence and phosphorescence, filter flurometers, spectroflurometrs. Photochemical kinetics of unimolecular and bimolecular processes. Quenching-collisions in the gas phase, solution (Stern-Volmer equation) & by added substances.

Photosensitized Reactions: Types-Photo-dissociation, Isomerisation and rearrangement reactions with specific examples. A brief introduction to some current topics in photochemistry - solar energy utilization. Photochemical devices. Photgalvanic cell, water splitting

REFERENCES:

1. Essentials of Nuclear Chemistry, H.J.Arnikar, New Age International Publishers, 2011.
2. Fundamentals of Photochemistry, Rohatgi and Mukherje,1stEdn,New Age International Publishers, 2006.
3. Principles of Instrumental Analysis, Skoog, Holler & Nieman, 6thEdn, Cengage India Pvt Ltd, 2008.
4. Instrumental methods of analysis, H.H. Willard, L.L. Merrit & J.J. Dean, 7thEdn,CBS Publishers,2012.
5. Analytical Chemistry: Principles, J.H. Kennedy, Cengage India Pvt Ltd,2011.
6. Advanced Organic Chemistry- Part A &B, Carrey & Sundberg,5thEdn,Springer 2007.
7. Organic Reaction Mechanisms, V. K. Ahluwalia, Rakesh Kumar Parashar,4thEdn, Narosa Publishing House Pvt Ltd, 2011.
8. Essentials of Molecular Photochemistry, A. Gilbert and J. Baggot, CRC Press, 1991.
9.Handbook of Photochemistry, S. Murov, I. Carmichael and G. L. Hug, Marcell Dekker,1993.
10. Principles of Molecular Photochemistry: An Introduction, N. J. Turro, V.Ramamurthy and J.C. Scaiano, University Science Books: Mill Valley, CA, 2008.

PH 583.4: CHEMISTRY OF POLYMERS AND NATURAL PRODUCTS

Course outcomes:

Student will be able to:

- Understand preparation methods, property uses of some industrially important polymers.
- Describe the morphology, structure thermal, physical, and mechanical properties of polymers.
- Gather knowledge about the classification, isolation techniques, understand the various synthetic approaches in Natural Products synthesis structural elucidation of natural products.
- Explain the basics and applications of concerted reactions and pericyclic reactions. Develop an in-depth knowledge of the basics and applications with mechanistic understanding in concerted reactions apply those in the synthesis of organic compounds.

UNIT I: **14 hours**

Definition of basic terms: Monomers, repeat units, degree of polymerization and Classification of polymers.

Polymer synthesis: Chain growth polymerization and step growth growth-radical-anionic-cationic-ring opening metathesis polymerization (ROMP), Polymerization techniques- Bulk, solution, suspension and emulsion polymerizations

Isolation and purification: Fractional precipitation, partial dissolution, gradient elution and Gel permeation chromatography.

Structure and Properties: Molecular weight and size, polydispersity and average molecular weight concept- Number, weight and viscosity average molecular weight concepts. Crystallinity requirements for crystallisability, effect of crystallinity on the properties of polymers. Mechanical properties: Tensile impact, flexural, and impact strength.

UNIT II : **14 hours**

Empirical formula, Molecular formula and methods to determine the molecular mass of a compound.

Determination of molecular weights - End-group analysis, viscosity, osmometry, and sedimentation method.

Thermal characterization: Glass transition temperature, Tg-transitions and associated properties, factors affecting the temperature and importance of Tg. Thermogravimetric analysis, and differential scanning calorimetry. Thermal stability, melting and thermal degradation temperatures..

Polymer Processing Techniques: Plastics - elastomers - fibres - film casting- compression moulding - injection moulding - blow moulding - extrusion moulding, elastomer properties, vulcanization, reinforcement, fillers, plasticizers and other additives.

UNIT III **14 hours**

History of Total Synthesis, Natural Product Chemistry.

Alkaloids: Definition, Classification and isolation of alkaloids, general methods of structural determination of alkaloids, detailed study of structure elucidation, stereochemistry, rearrangement, Synthesis and biogenesis of the following alkaloids- Papaverine, Quinine, Morphine, Codeine, Thebaine and Reserpine.

Terpenoids: Introduction, classification, isoprene rules, methods of structure determination. Structural elucidation & synthesis of Menthol, α-Pinene and Abietic acid

Unit IV **14 Hours**

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system.

Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions, conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloaddition reactions: antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 -dipolar cycloadditions and cheletropic reactions. Sigmatropic rearrangements: suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3- and sigmatropic rearrangements. Claisen and Cope rearrangements. Fluxional tautomerism. Ene reaction.

REFERENCES:

1. Polymer synthesis: A theory and practice-fundamentals, methods, experiments,*DBraun*, H Cherdron, M Rehahn, H Ritter and B Voit, 4th Edn,Springer, 2004.

2. Polymers: Chemistry and Physics of modern materials, *Cowie, J.M.G.* and Arighi, V., 3rd Edn, CRC Press, Boca Raton, FL, 2008.

3. Polymer Science and Technology, Plastics, Rubbers, Blends and composites, Premamoy G, 2nd Edn, Tata McGraw-Hill, New Delhi, 2003.

4. Polymer Science, V. R. Gowarikar, N. V. Viswanathan and J. Sridhar, New Age International, 2005.

5. Organic Chemistry-Vol-I,II, I.L.Finar, Longmann ELBS London, 2000.

6. Text Book of Polymer Science, F.W. Billmeyer, Wiley, New York, 2007.

7. *Contemporary polymer chemistry*, Harry Allcock, Pearson Higher Education &

professional Group, 2007.

8. The Chemistry of Polymers, John W. Nicholson, Royal Society of Chemistry, Cambridge CB4, 0WF, UK, 2012.

9. Advanced polymer chemistry, Selvaraj V.K, Campus Books International, New Delhi, 2012.

10. Natural Products Chemistry Vol-I&II, O. P. Agarwal, 42nd Edn, Krishna Prakashan, 2011.

11. Natural Products, Sujatha V Bhat and Nagasampige, 1st Edn, Springer, 2008.

12. Organic Chemistry, Jonathan Clayder, Greeres and Warren, 2nd Edn. 2001.

13. Mechanism of Organic Reactions, K.S Mukherjee, 2010.

PS 584.4P ORGANIC CHEMISTRY PRACTICALS – IV

Course outcomes:
Student will be able to:

- Detail the various organic reactions and their synthetic procedures.
- Analyze the separation processes of various organic compound mixtures and their quality checking processes

Multi Step Organic Synthesis

1. Ethyl resorcinol from Resorcinol
2. 3-Bromo-4-methyl benzaldehyde from p-Toluidine
3. ε-Caprolactam from cyclohexanone
4. p-Amionobenzoic acid from p-Nitrotoluidine
5. s-Tribromobenzene from aniline
6. o-hydroxy acetophenone from phenol
7. Benzanilide from Benzophenone
8. Benzylic acid from Benzoin
9. Benzopinacolone from Benzophenone
10. p-Chlorotoluine from p-Toluidine
11. 2,5-Dihydroxy acetophenone from Hydroquinone
12. 2,4-Dinitrophenylhydrazine from Chlorobenzene
13. m-Nitrobenzoic acid from Benzoic acid
14. 2,4-Dinitrophenol from Chlorobenzene
15. o-Aminobenzoic acid from Phthalic anhydride
16. 2-Carbethoxycyclopentanone from Adipic acid
17. α-Acetylamino cinnamic acid from Glycine
18. p-Aminoazobenzene from Aniline.
19. Separation of components from mixture of organic compounds by fractional crystallization, fractional distillation, adsorption, Paper and TLC.Their purification and characterization.

REFERENCES :

1. Practical Organic Chemistry, F .G. Mann and B. C. Saunders, Universities Press, 2004.
2. Practical Organic Chemistry, A. I. Vogel, 5thEdn, Pearson, 2005.
3. Experimental Organic Chemistry–Vol.I&II, Singh et al, Campus Book International.
4. Vogel's Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis, B. S. Furniss et al, 2ndEdn, Pearson Education, 1989.

PS 585.4P : INORGANIC CHEMISTRY PRACTICALS – IV

Course outcomes:
Student will be able to:

- Estimate binary mixtures of metallic ions in solution.
- Study structure of the prepared complexes using conductance and magnetic susceptibility measurements, recording the electronic and infrared spectra:

Inorganic Practicals :

1. Colorimetric determination of Ti(IV) and Zr(IV)
2. Circular paper chromatography-separation of -

a) iron and nickel; b) copper and nickel; c) copper, cadmium and mercury

3. Thin layer chromatographic separation of amino acid
4. Separation and determination of cadmium and zinc on an anion- exchanger.
5. Separation of Cobalt and Nickel by column chromatography
6. Separation of Nickel, Manganese, Cobalt and Zinc by paper chromatography
7. Simultaneous colorimetric determination of two metal ions – Mn and Cr.
8. Flame photometric determination of Na, K, Li and Ca individually and in mixtures.
9. Electrogravimetric determination of (a) Cu-Ni alloy and (b) Pb in Type Metal.
10. Solvent extraction of Ni(II) and UO_2(II).
11. Preparation of any three of the following complexes, checking the purity of the prepared samples by chemicals analysis, structural study of the prepared complexes using conductance and magnetic susceptibility measurements, recording the electronic and infrared spectra:

a. Chloropentamminecobalt(III) chloride
b. Hexamminecobalt(III)chloride.
c. Potassium trisoxalatoferrate(III)
d. Potassium hexathiocyanatochromate(III)
e. $K_3Cr(OX)_3.3H_2O$

12. Determination of composition of complexes:

a. Job's method: Fe-phenanthroline complex
b. Mole ratio method: Zr-Alizarin red S complex,
c. Slope ratio method: Cu ethylenediamine complex,
d. Limiting logarithmic method: Uranyl-sulphosalicyclic acid complex.

13. Determination of stability constants

a. Turner Anderson method : Fe-Tiron system,
b. Bejrrum's method : Cu – sulphosalicyclic acid system,
c. Polarographic method : Cu-glycinate or Pb -oxalate system.

REFERENCES :

1. A Text Book of Quantitative Inorganic Analysis, A.I. Vogel, 4thEdn, Longmann Science and Tech,1980.
2. Vogel's Text Book of Quantitative Inorganic Analysis, Basset, Denney, Jeffery & Mendham, 6thEdn, Pearson, 2011.
3. Practical Inorganic Chemistry, G. S Turpin, Hardpress Publishing, 2012.
4. Practical Inorganic Chemistry, Navneet Manav, Amita Dua, Manakin Press, 1st, 2017.

PH 586.4 PROJECT WORK

PS 587.4 : SOLID STATE AND NANO CHEMISTRY

Course Outcome:
Student Will be able to:

- Understand the theory of diffraction techniques
- Gain a domain knowledge about crystal systems and defects
- Understand the importance and basic concepts of Nano Chemistry

UNIT I **14 Hours**

Types of crystalline solids, types of crystal lattices, unit cell, space lattice, co-ordination number, calculation of number of particles in unit cell& types of close packing.

Diffraction Techniques: X-ray diffraction: Bragg condition, Miller indices, Laue method, Bragg method, Debye-Scherrer method, method of X-ray structural analysis, X-rays - charecteristics, Generation of X-rays, X-ray absorption, Theoretical Background of Diffraction, Diffraction Geometry, Reciprocal Lattice

Interpretation of powder patterns.Film method (Weissenberg method). X-ray diffractometers. Systematic absences. Intensities of diffracted X-rays and structural analysis, X-ray scattering by atoms and molecules, Factors affecting X-ray intensities.

Electron Diffraction: Scattering intensity and scattering angle, Wierl equation, measurement technique, electron diffraction of gases and molecules, Low Energy Electron Diffraction and structure of surfaces.

UNIT II **14 Hours**

Defects in crystal system, point, line and plane defects, stoichiometric and non-stoichiometric defects.

Crystal Defects and Non-Stoichiometry: Perfect and imperfect crystals, intrinsic and extrinsic defects, Concentration of defects Vacancy, Schottky and Frenkel defects. Thermodynamics of Schottky and Frenkel defect formation, colourcentres, non-stoichiometry defects – Structures of UO_2, FeO and TiO.. Ionic conductivity in solids, solid electrolytes, fast-ion conductors: oxygen and sodium ion conductors. Applications of solid electrolytes: 1) fuel cells, 2) sensors, 3) electro chromic devices, ~~nonstoichiometric compounds, introduction.~~

Preparative Methods: Ceramic, sol-gel, precursor and chemical vapor deposition (CVD) methods. Nucleation & crystal growth techniques-pulling, zoning, flame fusion & skull melting. Basic methods of preparation of thin films.

Electronic Properties of solids: Electrical conductivity, Hall effect. Metals, Insulators and Semiconductors.Intrinsic and extrinsic semiconductors, hopping semiconductors.Metal–semiconductor and p-n junctions.Dielectric, ferroelectric, pyroelectric & piezoelectric properties & their applications. Superconductivity: Introduction, Discovery, Effect of magnetic field on Superconductors

UNIT –III: **14 Hours**

Nano materials, history, defining nano dimensions, scope of nano materials.

Nano structures: self assembly - nano particles, methods of synthesis- sol-gel process, electrodeposition, chemical vapour deposition, co-precipitation, hydrothermal synthesis, hydrolysis of salts and alkoxides. Electrokinetic potential and peptization reactions- gelation network-xerogels, aerogels- drying of gels, chemical nanocomposites, consumer goods, ‘smart materials,’

Properties of materials & nanomaterials, role of size and shape in nanomaterials
Brillouin zones, Mobility, Resistivity. Magnetic Properties: Superparamagnetism, blocking. Important properties in relation to nanomagnetism
Applications to various fields: Nano electronics, nano medicine, nano photonics, nano spintronics, nano materials in catalysis.

REFERENCES:

1. Electronic absorption Spectroscopy and Related Techniques, D.N.Satyanarayana,1st Edn, Universities Press, 2000.
2. Inorganic Chemistry, Huheey, Kieter, Medhi, 4th Edn, Pearson, 2011.
3. Solid State Chemistry and its applications, A.R.West,1st Edn, Wiley India Pvt Ltd, 2003.
4. Principles of Solid State, H. V. Keer, New Age International Publishers Pvt Ltd.
5. Solid State Physics, S. O. Pillai, New Age International Publishers Pvt Ltd.
6. Material Science and Engineering: An Introduction, W. D. Callister, 6th Edn, Wiley, 2002.
7. Klabunde, K. J., Ed. Nanoscale Materials in Chemistry, Wiley Interscience (2001)
8. Kulkarni, S. K. Nanotechnology: Principles and Practices, Capitol Publishing Company (2007)
9. Wilson, M., Kannangara, K., Smith, G., Simmons, M. & Raguse, B. Nanotechnology: Basic Science and Emerging Technologies, Overseas Press (2005).
10. Poole Jr., C. P. & Ovens, F. J. Introduction to Nanotechnology, Wiley Interscience (2003)
11. Edelstein, A.S. & Cammarata, R. C., Ed. Nanomaterials: Synthesis, Properties and Applications, Institute of Physics Publishing (1996) 28
12. Rao, C.N.R., Müller & Cheetham, A.K., Eds. The Chemistry of Nanomaterials: Synthesis, Properties and Applications, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim (2004)
13. Edelstein, A.S. & Cammarata, R.C., Ed. Nanomaterials: Synthesis, properties and Applications, Institute of Physics Publishing (1996).
14. Moore, E. & Smart, L. Solid State Chemistry: An Introduction 2nd Ed. Chapman & Hall (1996)
15. Rhodes, G. Crystallography Made Crystal Clear: A Guide for Users of Macromolecular Models 3rd Ed. Elsevier (2006)
16. Massa, W. Crystal Structure Determination 2nd Ed. Springer (2004).
17. Warren, B. E., X-Ray Diffraction 1st Ed. Dover Publications (1990). 5. Sands, D. E. Introduction to Crystallography Reprint Dover Publications (1994)

PS 588.4 :OPTICAL METHODS OF ANALYSIS

UNIT I: **14 hours**

Basics of emission, absorption, instrumentation and principle of spectrophotometer.

Atomic emission spectroscopy and atomic absorption spectroscopy- Introduction, principle, flames and flame spectra, variation of emission intensity with the flame, flame temperature, chemical reactions in flame, metallic spectra in flame, flame background. Total consumption and premix burners, role of temperature on absorption, emission and fluorescence.Effect of organic solvents.Comparative study of the basic components and difference in the instrumental design for atomic absorption, atomic fluorescence and flame photometry.Errors in flame photometry (interferences).Precision and accuracy of AAS and FES. Relationship between AAS and FES, advantages over FES, devices used for the formation of an atomic vapor, Plasma excitation sources, applications, determination of sodium in different samples by flame photometry. Some typical determinations by atomic absorption spectroscopy.

UNIT II: **14 hours**

Phenomenon of fluorescence, phosphorescence, Quantum yield.

Molecular Luminescence: Fluorimetry and phosphorimetry, Introduction, fluorescence and phosphorescence, factors affecting fluorescence and phosphorescence, Jablonski Diagram, internal conversion, intersystem crossing (radiationless processes), quenching. Theory, relationship between intensity of fluorescence and concentration, instrumentation-basic differences in the measurement of fluorescence and phosphorescence, filter fluorimeters, spectrofluorimeters, advantages, limitations and precautions. Selection of excitation wavelength for analysis, reporting fluorescence spectra.Application of fluorimetric analysis of inorganic, organic, pharmaceutical, agricultural, biochemical and biomedical materials.Special fluorimetric and phosphorimetric applications. Chemiluminescence

UNIT III **14 hours**

Phenomenon of optical activity, plane polarised light, instrumentation and working of polarimeter. Comparison of spectrophotometer and colorimeter.

Nephelometry and Turbidimetry: Light scattering, nephelometry and turbidimetry, choice between nephelometry and turbidimetry, turbidimetry and colorimetry, nephelometry and fluorometry. Theory, effects of concentration, particle size and wavelength on scattering instruments and application of nephelometry and turbidimetry. Turbidimetric titrations.

Polarimetry: Instrumentation, optical rotatory dispersion(ORD). Application of optical rotation method in the determination of rate constant.Acid-catalyzed mutarotation of glucose, inversion of cane sugar- Relative strengths of acids.Circular Dichroism and its applications, deduction of absolute configuration of molecules, octant rule for ketones and cotton effect.

REFERENCES

1. Fundamentals of Analytical Chemistry, S.A. Skoog, 9th Edn, Cengage Learning, 2014.
2. Basic concepts of Analytical Chemistry, S. M. Kopkar, 3rd Edn, New Age International, 2009.
3. Quantitative analysis, Day & Underwood, 6th Edn, PHI Learning, 2015.
4. Vogel's Text book of Quantitative Chemical Analysis, Bessett, Denney, Jeffery & Mendham, 7th Edn, Pearson, 2013.
5. Principles of Instrumental Analysis- Skoog, Holler & Nieman, 8th Edn. Cengage, 2012.
6. Instrumental methods of analysis, H.H. Willard, L.L. Merrit & J.J. Dean, 7th Edn, CBS Pubs, 2012.
7. Analytical Chemistry: Principles, J.H. Kennedy, 2nd Edn, Cengage, 2011.
8. Analytical Chemistry, G.D. Christian, 6th Edn, Wiley, 2015.
9. Chemical Analysis-An Instrumental Approach- Srivastava & Jain, 4th Edn, S.Chand, 2015.
10. Instrumental methods of Chemical Analysis-Gurdeep R Chatwal, 5th Edn, Himalaya Publishing House, 2015.
11. Fundamentals of photochemistry, Rohatgi and Mukherjee, New Age, 2014.

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