St. PETER'S UNIVERSITY

St. Peter's Institute of Higher Education and Research
(Declared Under Section 3 of the UGC Act, 1956)
AVADI, CHENNAI – 600 054
TAMIL NADU

M.Sc. (CHEMISTRY)
Code No. – 418
(Effective From **2009 – 2010**)
(Distance Education)

Regulations and Syllabi
(I & II Year)

St. PETER'S INSTITUTE OF DISTANCE EDUCATION
Recognized by Distance Education Council and
Joint Committee of UGC – AICTE - DEC, New Delhi
(Ref. F. No. DEC/SPU/CHN/TN/Recog/09/14 dated 02.04.2009 and Ref.F.No.DEC/Recog/2009/3169 dated 09.09.2009)

St. PETER'S UNIVERSITY

St. PETER'S INSTITUTE OF DISTANCE EDUCATION

Chennai – 600 054.

Code No. – 418

M.Sc. (CHEMISTRY)

(Distance Education)

Regulations and Syllabi

(Effective from 2009 – 2010)

1. **Eligibility:** A Candidate who has passed B.Sc. Examination with Chemistry as main subject of study or any of the B.Sc. Degree Examination with specialization such as Industrial Chemistry, Applied Chemistry, or any other specialization in Chemistry of other University recognized by this University as equivalent thereto, are eligible for admission to Two Year M.Sc. Programme in Chemistry.

2. **Duration:** Two Years.

3. **Medium:** English is the medium of instruction and examination.

4. **Methodology:** The methodology of distance education includes the supply of self-instructional study materials in print format and in CD, face-to-face instruction for theory and practicals for a limited period during week ends and on holidays, provision of virtual class in phased manner, dissemination of information over e-mail, Student - Support Service at various Centres of the University, Continuous Assessment and End Assessment conducted by the University at various parts of India.

5. **Weightage for Continuous and End Assessment:** There is no weightage for Continuous Assessment unless the ratio is specifically mentioned in the scheme of Examinations. The End Assessment (EA) has 100% weightage.

6. Credit System: Credit system be followed with 36 credits for each Year and each credit is equivalent to 25 hours of effective study provided in the Time Table of the formal system.

7. Scheme of Examinations

First Year

Code No.	Course Title	Credit	Marks	
Theory			**EA**	**Total**
109PCHT01	Organic Chemistry I	4	100	100
109PCHT02	Inorganic Chemistry I	4	100	100
109PCHT03	Physical Chemistry I	3	100	100
109PCHT04	Polymer Chemistry	3	100	100
109PCHT05	Spectroscopy - I	3	100	100
109PCHT06	Nano materials and Green Chemistry	4	100	100
109PCHP01	Practical I-Organic Chemistry-I Record	5	90 10	100
109PCHP02	Practical II-Inorganic Chemistry-I Record	5	90 10	100
109PCHP03	Practical III-Physical Chemistry-I Record	5	90 10	100
	Total	**36**	**900**	**900**

Second Year

Code No.	Course Title	Credit	Marks	
Theory			**EA**	**Total**
209PCHT01	Organic Chemistry II	4	100	100
209PCHT02	Inorganic Chemistry II	4	100	100
209PCHT03	Physical Chemistry II	4	100	100
209PCHT04	Photo Chemistry	3	100	100
209PCHT05	Spectroscopy - II	3	100	100
209PCHT06	Environmental Chemistry	3	100	100
209PCHP01	Practical IV-Organic Chemistry-II Record	5	90 10	100
209PCHP02	Practical V-Inorganic Chemistry-II Record	5	90 10	100
209PCHP03	Practical VI-Physical Chemistry-II Record	5	90 10	100
	Total	**36**	**900**	**900**

8. Passing Requirements: The minimum pass mark (raw score) be 50% in End Assessment.

9. Grading System: Grading System on a 10 Point Scale be followed with 1 mark = 0.1 and the conversion of the Grade point as given below.

$$\text{Overall Grade Point Average (OGPA)} = \frac{\text{Sum of Weighted Grade Points}}{\text{Total Credits}}$$

$$= \frac{\Sigma\,(EA)C}{\Sigma C}$$

10. The Overall Grade: The Overall Grade and Classification of all successful candidates be arrived at from the Overall Grade Point Average as stipulated in the following conversion Table.

Grade	Over all Grade Point Average(OGPA)	Over all weighted Average marks	Classification
0	9.0 to 10.0	90 to 100	First Class
A	8.0 to 8.9	80 to 89	First Class
B	7.0 to 7.9	70 to 79	First Class
C	6.0 to 6.9	60 to 69	First Class
D	5.0 to 5.9	50 to 59	Second Class
F	0.0 to 4.9	0 to 49	**Reappearance**

The Grade Sheets of successful candidates provide particulars such as (1) Overall weighted Average Marks and (2) Overall Grade.

11. Pattern of the Question Paper: The question paper for the End Assessment will be set for three hours and for a maximum of 100 marks with following divisions and details.

Part A: 10 questions (with equal distribution to all the units in the syllabus). Each question carries 2 marks.

Part B: 5 questions with either or type (with equal distribution to all the units in the syllabus). Each question carries 16 marks.

The total marks scored by the candidates will be calculated to the maximum prescribed in the Regulations.

12. Syllabus

109PCHT01: ORGANIC CHEMISTRY – I

UNIT – I: Types of Reactions, Mechanisms and Reaction intermediates

Types of reactions : Substitutions, Additions, Eliminations, Rearrangements, Oxidations and Reductions reactions – a general study.

Reaction mechanisms: Types of mechanisms: Heterolytic, Homolytic and Pericyclic mechanisms – a general study.

Reaction intermediates:_Formation, stability and structure of carbonium ions, carbanions, carbenes, nitrenes and free radicals.

Long lived and short lived free radicals, methods of generation and detection of free radicals, free radical reactions: Sandmeyer reaction, Gomberg-Bachmann reaction, Pschorr reaction and Ullmann reaction, mechanism of Hunsdiecker reaction.

UNIT – II: Stereochemistry

Concept of chirality, recognition of symmetry elements and chiral structures, R – S nomenclature, Fischer, Newman and Sawharse projections of erythro and threo forms of organic molecules and their interconversion. Optical activity in the absence of chiral carbon – biphenyls, allenes and spiranes – R and S notations. Chirality due to helical shape, trans cyclooctene, cyclononene. E – Z isomerism of olefins containing one double bond . Stereochemistry and Conformational Analysis : Stereospecific and stereoselective synthesis with one suitable example, asymmetric synthesis – Crams rule, Conformational analysis and stereochemical features of disubstituted cyclohexanes (1,2 ; 1,3 ; 1,4 dialkyl cyclo hexanes), conformation and stereochemistry of cis and trans decalins,

UNIT – III: Aliphatic Nucleophilic Substitution Reactions

The S_N^2, S_N^1,mixed S_N^1 and S_N^2, S_N^i and SET mechanisms. The neighbouring group mechanism, neighbouring group participation by π and σ bonds, anchimeric assistance. Nucleophilic substitution at an allylic, aliphatic trigonal and vinylic carbon.

Reactivity effects of substrates structure, attacking nucleophile, leaving group and reaction medium, ambident nucleophile, regioselectivity. Substitution at carbon doubly bonded to oxygen and nitrogen, Williamson reaction, Von-braun reaction, hydrolysis of esters, Claisen and Dieckmann condensation.

UNIT IV: Heterocyclic Compounds

Synthesis and properties of imidazole, oxazole, thiazole and indole.

General methods of Synthesising Anthocyanidins, Synthesis and Structural elucidation of Cyanidin Chloride, Synthesis and Structural elucidation of flavones and isoflavones (Daidzein), Synthesis of pyrimidine and its derivativess, Synthesis of purine, uric acid and caffeine).

UNIT V: Aromatic electrophilic, nucleophilic substitution reactions and Aromaticity

The arenium ion mechanism, typical reactions like nitration, sulphonation, haloganation, Friedal-Crafts alkylation, acylation and diazonium coupling, electrophilic substitution on monosubstituted benzene, orientation and reactivity-ortho, meta and para directing groups, Gatterman, Gatterman-koch, Vilsmeir, Reimer-Tiemann reaction.

Aromatic nucleophilic substitution reactions, the S_NAr, mechanism, aromatic nucleophilic substitution of activated halides-Ziegler alkylation, Chichibabin reaction.

Aromaticity of benzenoid, heterocyclic and non-benzenoid compounds, Huckel rule, aromatic systems with pi electron compounds other than six pi electrons, non-aromatic (cyclooctatetraene, etc.,) and anti aromatic systems (cyclobutadiene, etc.,), systems with more than 10 pi electrons.

Text Books

1. Jerry March, **Advanced Organic Chemistry**- Reactions, Mechanisms and Structure, Fourth Edition, John Wiley & Sons (1992).
2. Francis A. Carey, **Organic Chemistry**, Third Edition, The McGraw-Hill Companies, Inc., 1996.
3. P. S. Kalsi, Organic Reactions and Mechanisms, Second Edition, New Age International Publishers, 2002.
4. Ernest L. Eliel, **Stereochemistry of Carbon Compounds**, T.M.H Edition, Tata McGraw-Hill Publising Company, 1995.

5. P. S. Kalsi, **Stereochemistry – Conformation and Mechanism**, 6th Edition, Wiley Eastern Limited, 2005.
6. I.L. Finar, **Organic Chemistry**, Volume. II, Fifth Edition, First Indian reprint, Pearson Education Asia Pte. Ltd., (2000).

Reference Books

1. P.S. Kalsi, **Stereochemistry and Mechanism through solved problems**, Second Edition, New Age International Publishers, 1994.
2. D. Nasipuri, **Stereochemistry of Organic Compounds**, 2nd Edition, New Age International Publishers, 1994.
3. S.M.Mukherji and S.P.Singh, **Reaction Mechanism in Organic Chemistry**, 1st Edn., Macmillan 1976.
4. R.T.Morrison and R.N.Boyd, **Organic Chemistry,** 6th Edn., Prentice-Hall,1992.
5. R.O.C. Norman, **Principles of Organic Synthesis**, Second Edition, Chapman and Hall, 1978.
6. R.M.Acheson, **Introduction to Chemistry of Heterocyclic Compounds**, 2nd Edn., Interscience Publishers, 1967.
7. J.A. Joule and G.F. Smith, **Heterocyclic Chemistry**, Van Notrand Reishord Co., London, 1978.

109PCHT02: INORGANIC CHEMISTRY - I

UNIT I : Structure and Bonding

Van der Waals bonding, Hydrogen bonding and applications, Hard and Soft acids and bases-classification, Acid-Base strength, hardness, Symbiosis, Theoretical basis of Hardness and Softness, applications of HSAB.

Polyacids - Isopolyacids of V, Cr, Mo and W; Heteropolyacids of Mo and W (only structural aspects).

Inorganic polymers – Silicates – structure, Pauling's rule, properties, correlation and application; Molecular sieves.

Rings – Phosphazenes – Structure, Craig and Peddock model, Dewar model, polyorganophosphazenes, Polysulphur-nitrogen compounds.

UNIT – II: Nuclear Chemistry

Nuclear properties - Nuclear spin and moments, origin of nuclear forces, features of the liquid drop and the shell models of the nucleus; Modes of radioactive decay - orbital electron capture, nuclear isomerism, internal conversion; Detection and determination of activity - Cloud chamber, nuclear emulsion, Bubble chamber, GM, Scintillation and Cherenkov counters.

Nuclear reactions - Types, reaction cross section, Q-value, threshold energy, compound nuclear theory, high energy nuclear reactions, nuclear fission and fusion reactions as energy sources, direct reactions, photonuclear and thermo nuclear reactions, Stellar energy, synthesis of elements.

Applications relating to Nuclear Chemistry - Neutron activation analysis, Radio pharmacology, Radiation protection and safety precautions, Isotope dilution analysis.

Radiation Chemistry - Range of alpha and beta radiations, radiation dosimetry, radiolysis of water, the hydrated electron.

UNIT III: Stability and bonding in complexes

Stability of complexes -Factors affecting stability of complexes, thermodynamic aspects of complex formation, Stepwise and overall formation constants, stability correlations,

statistical and chelate effects; Determination of stability constant - polarographic, photometric and potentiometric methods.

Stereochemical aspects - Stereoisomerism in inorganic complexes, isomerism arising out of ligand distribution and ligand conformation, chilarity and nomenclature of chiral complexes; application of ORD and CD in the identification of chirality of complexes.

Macrocyclic ligands - types - porphyrins, corrins, Schiff's bases, crown ethers and cryptates. (simple complexes)

Metal-Ligand Bonding Crystal field theory - Splitting of d- orbitals under various geometries, factors affecting splitting, CFSE, evidences for CFSE (Structural and thermodynamic effects), Spectrochemical series, Jorgensen relation, site preferences; Jahn-Teller distortion - Splitting pattern in trigonal pyramid, square pyramidal and cubic symmetries, Dynamic and Static J.T. effect, Jahn-Teller effect and Chelation; Limitations of CFT; Evidences for metal-ligand overlap; M.O. theory and energy level diagrams, concept of weak and strong fields, sigma and pi bonding in complexes, nephelauxetic eff

UNIT IV: Electronic Spectra of Complexes

Spectroscopic Term symbols for d^n ions - derivation of term symbols and ground state term symbol, Hund's rule; Selection rules – break down of selection rules, spin- orbit coupling, band intensities, weak and strong field limits- correlation diagram; Energy level diagrams; Orgel and Tanabe-Sugano diagrams; effect of distortion and spin orbit coupling on spectra; Evaluation of Dq and B values for octahedral complexes of Nickel; Charge transfer spectra; , magnetic properties of complexes.

UNIT V: Analytical Chemistry

Polarography - Theory, apparatus, DME, diffusion, kinetic catalytic currents, current voltage curves for reversible and irreversible systems; qualitative and quantitative applications to Inorganic systems.

Amperometric titrations - Theory, apparatus, types of titration curves, successive titrations and two indicator electrodes; applications; Complexometric titrations - Chelating agents; types of EDTA titration - direct and back titrations; replacement titrations - masking and demasking reagents.

Chromatography - Gas liquid chromatography – principle; retention volumes; instrumentation; carrier gas; columns preparations; stationary phase; detectors - thermal conductivity, flame ionization, electron capture; applications of GLC.

High performance liquid chromatography – scope; column efficiency; instrumentation; pumping systems; columns; column packing; detectors; applications.

Text Books :

1. H.J. Emelius and Sharpe, **Modern aspects of Inorganic chemistry,** Universal book Stall, New Delhi, 1989.
2. J.E. Huheey, E.A. Keiter and R.L. Keiter, **Inorganic Chemistry- Principles of structure and reactivity**, 4th edition, Pearson-Education, 2002.
3. F.A. Cotton and G. Wilkinson, **Advanced Inorganic Chemistry,** Wiley Eastern, 5th edition, 1988.
4. F. Basolo and R.G. Pearson, **Mechanism of Inorganic Reactions**, Wiley Eastern, 1967.
5. S. Glasstone, **Source book of Atomic Energy**, Van Nonstrand Co., 1969.
6. H.J. Arniker, **Essentials of nuclear chemistry**, 2nd edition Wiley eastern Co.,1987.
7. D.A. Skoog, **Principles of Instrumental Analysis**, Saunders College Pub.Co, III Edn., 1985.
8. J.G. Dick, **Analytical Chemistry**, McGraw Hill Publishers, 1974.
9. A.I Vogel, **Text Book of Quantitative Inorganic Analysis**, Pearson V Edn., 2001.
10. R.C. Kapoor and B.S. Agarwal, **Principles of polarography**, Wiley Eastern Ltd., 1991.

Reference Books

1. K.F. Purcell and J.C. Kotz, **Inorganic Chemistry,** WB Saunders Co. USA 1977.
2. G.S. Manku, **Inorganic Chemistry,** TMH Co., 1984.
3. A.K. Srivatsava and P.C. Jain, **Elements of Nuclear Chemistry,** S. Chand and Co., 1989.
4. G. Friedlander, J.W. Kennedy and J.M. Miller, **Nuclear and Radiochemistry,** Wiley, 1964.
5. Willard, Merit, Dean and Settle, **Instrumental Methods of Analysis**, CBS Publishers and Distributors, IV Edn.,1989
6. G. D. Christian and J.E.O Reilly, **Instrumental Analysis**, Allyn and Bacon Inc, II Edn., 1986.

109PCHT03: PHYSICAL CHEMISTRY – I

UNIT- I: Classical Thermodynamics –I

Maxwell's relations and thermodynamic equations of state – applications in the evaluation of Cp – Cv for solids and for vanderwaals gases, Cp – Cv in terms of coefficient of expansion and coefficient of compressibility – Relation between Cp and Cv – Partial molar properties- Gibbs – Duhem equation- Partial molar free energy (Chemical Potential) – Determination of chemical potential [Direct method and Method of Intercepts] and partial molar volume – variation of chemical potential with Temperature and Pressure – Thermodynamic derivation of phase rule – application to three component systems involving solids and liquids (CH_3 COOH – $CHCl_3$ – H_2O, NaCl – Na_2SO_4 - H_2O and NH_4 NO_3 –$(NH_4)_2$ SO_4 – H_2O).

UNIT –II: Statistical Thermodynamics

Objectives of Statistical Thermodynamics – concept of thermo dynamical and mathematical probabilities – Distribution of distinguishable and non- distinguishable particles.

Maxwell – Bottzmann, Bose – Einstein and Fermi – Dirac statistics – comparison and application.

Partition Functions – evaluation of Translational, Vibrational, Rotational and Electronic partition Function – Thermodynamic Functions in terms of partition Function – Application of Partition Function to monatomic and diatomic gases – Statistical expression for equilibrium Constant – Calculation of Equilibrium Constant from Partition Function – (isotope exchange equilibrium and dissociation of diatomic molecules) – Heat capacities of Monatomic crystals – Einstein and Debye theory of heat capacities.

UNIT –III: Group Theory –I

Symmetry elements and symmetry operations – Point groups – identification and representation of groups – comparison of Molecular symmetry with Crystallographic

symmetry – Reducible and irreducible representation – Direct product representation – Great orthogonality theorem and its consequences – Character Table and their uses.

UNIT –IV: Group Theory – II

Symmetry selection rules for vibrational, Electronic and Raman Spectra – determination of representation of vibrational modes in non- linear molecules such as H2O, CH4, XeF4, SF6 and NH3 – symmetry of Hybrid orbitals in non- linear molecule (BF3, CH4, XeF4, PCl5, and SF6,) – Electronic spectra of formaldehyde – application of group theory.

UNIT –V: Chemical Kinetics

Theories of Reaction rates – Arrhenius theory – effect of temperature on reaction rate – Hard – Sphere collision theory of reaction rates – molecular beams – collision cross section – effectiveness of collisions – Probability factor.

Transition state theory of reaction rates - Potential energy surface – Partion functions and activated complex – Eyring equation - Comparison of results with Eyring and Arrhenius equations – Estimation of free energy, enthalpy and entropy of activation and their significance.

Text Books :

1. S. Glasstone, **Thermodynamics for chemists**, Affiliated East West press, New Delhi, 1960.
2. J. Rajaram and J.C. Kuriacose, **Thermodynamics for students of Chemistry**, Lal Nagin Chand, New Delhi, 1986.
3. J. Rajaram and J.C. Kuriacose, **Kinetics and mechanism of chemical transformation** Macmillan India Ltd., 1993.
4. K.J. Laidlar, **Chemical kinetics**, Harper and Row New york, 1987.
5. D.A. Mcquarrie, **Quantum chemistry**, University science books, Mill Valley, California (1983)
6. R.K. Prasad, **Quantum Chemistry**, Wiley Eastern, New Delhi,1992.
7. V. Ramakrishnan and M.S. Gopinathan, **Group theory in Chemistry**, Vishal Publications, 1988.
8. K.V. Raman, **Group theory and its application to Chemistry**, Tata McGraw Hill Publishing Co., 1990.

Reference Books

1. W.J. Moore, **Physical Chemistr**y, Orient Longman, London, 1972.
2. K.G. Den Beigh, **Thermodynamics of Steady state**, Meklien and Co., London, 1951.
3. L.K. Nash, **Elements of Chemical Thermodynamics**, Addison Wesley, 1962.
4. R.G. Frost and Pearson, **Kinetics and Mechanism**, Wiley NewYork, 1961.
5. J.W. Moore and R.G. Pearson, K**inetics and Mechanism**,1981
6. C. Capellos and B.H.J. Bielski, **Kinetic Systems**, Willey Interscience, Newyork, 1968.
7. G.M. Harris, **Chemical Kinetics**, D.C. Heath and Co, 1966.
8. I.N. Levine, **Quantum Chemistry**, Allyn and Bacon, Boston, 1983.
9. J. Goodman, **Contemporary Quantum Chemistry, An Introduction**, Plenum Press, Newyork, 1977.
10. F.J. Bockhoff, **Elements of Quantum Theory**, Addision Wesley, Reading, Mass, 1976.
11. P.W. Atkins, **Physical Chemistry**, Oxford University press, Oxford. 1990.
12. P.W. Atkins, **Molecular Quantum Mechanics**, Oxford University press, Oxford, 1983.
13. H. Eyring, J, Walter and G. Kimball, **Quantum chemistry**, John Wiley and sons, Newyork, 1944.
14. L.S. Pauling and E.B. Wilsob, **Introduction to Quantum Mechanics**, McGraw Hill book co, Newyork, 1935.
15. F.A. Cotton, **Chemical Application of Group Theory**, John Wiley and sons Inc., Newyork, 1971.
16. N. Tinkham, **Group theory and Quantum Mechanics**, McGraw Hill Book Company, Newyork, 1964.
17. Alan Vincent, **Molecular Symmetry and Group theory –Programmed Introduction to chemical applications**, Wiley, Newyork, 1977.
18. G.M. Barrow, **Introduction to Molecular Spectroscopy**, McGrawhill, Newyork, 1962.
19. G.W. King, **Spectroscopy and Molecular Structure**, Holt, Rienehart and Winston, 1964.
20. E.B. Wilson, J.C. Decius and D.C. Cross, **Molecular Vibrations,** Mc Graw Hill Book Co.1955.
21. B.P. Straughan and S. Walker, **Spectroscopy** Vol - I, Vol- II and Vol-III, Chapmann and Hall, 1976

109PCHT04: POLYMER CHEMISTRY

UNIT I: Basic Concepts

Monomers, repeat units, degree of Polymerization, Linear, branched and network Polymers. Condensation Polymerization :Mechanism of stepwise polymerisation. Kinetics and statistics of linear stepwise polymerization. Addition polymerization: Free radical , cationic and anionic polymerization. Polymerization conditions. Polymerization in homogeneous and heterogeneous systems.

UNIT II: Co-ordination Polymerization

Kinetics, mono and bimetallic mechanism of co-ordination polymers.. Co-Polymerization: Block and graft co-polymers, Kinetics of copolymerization. Types of co-polymerization. Evaluation of monomer. Reactivity ratio. Rate of Co-Polymerization.

UNIT III: Molecular Weight and Properities

Polydispersion – average molecular weight concept, number, weight and viscosity average molecular weights. Measurement of molecular weights. Gel permeation chromatography, viscosity, light scattering, osmotic and ultracentrifugation methods. Polymer structure and physical properities – crystalline melting point T_m. The glass transition temperature. Determination of T_g . Relationship between T_m and T_g .

UNIT IV: Polymer Processing

Plastics, elastomers and fibres. Compounding processing techniques: calendering, die casting, rotational casting, film casting, injection moulding, blow moulding extrusion moulding, thermoforming, foaming, reinforcing and fibre spinning.

UNIT V: Properties of Commercial Polymers

Polyethylene, polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins and silicone polymers. Functional polymers – Fire retarding polymers and electrically conducting polymers. Biomedical polymers – contact lens, dental polymers, artificial heart, kidney, skin and blood cells.

Text Books

1. F.W. Billmeyer, **Text Book of Polymer Science**, 3rd Edn., J. Wiley, 2003.

2. V.R. Gowarker, N.V. Viswanathan and J. Sreedhar, **Polymer Science**, New Age Int.,1986.

Reference Books

1. H.R. Alcock and F.W. Lamber, **Contemporary Polymer Chemistry**, Prentice Hall,1981.
2. P.J. Flory, **Principles of Polymer Chemistry**, Cornell University press, New York, 1953.
3. G. Odian, **Principles of Polymerization**, 2nd Edn., John Wiley & Sons, New York,1981.

109PCHT05: SPECTROSCOPY – I

UNIT – I: Microwave Spectroscopy

Interaction of matter with radiation – Einstein's theory of transition probability – Rotation spectroscopy – Rigid Rotor – Intensity of spectral lines – Molecular parameters from Rotation spectra – Effect of isotopic substitution on the rotation spectra.

UNIT-II: IR and Raman Spectra

Theory, principle, instrumentation of IR and Raman Spectra. Characteristic group frequencies of organic molecule, Factors influencing vibrational frequencies, interpretation of IR spectra of organic molecules. Raman spectroscopy – Raman effect – Rotational and vibrational Raman Spectra. Applications of Raman Spectra.

UNIT-III: UV-VIS and Emission Spectra

Theory, principle, instrumentation of UV – VIS and Emission spectra.

UV-VIS: Woodward – Fieser rules for dienes, enones. Calculation of λmax for organic molecules. Chromophores and effect of conjugation, substituents with unshared electrons and their capability of π - conjugation . Colour in compounds.

Applications of UV – VIS and Emission spectra.

UNIT-IV: ^{1}H and ^{13}C NMR Spectra

NMR spectroscopy : Theory, principle, instrumentation, Chemical shift, factors influencing chemical shift, spin-spin coupling, NMR of simple AX and AMX type organic molecules, calculation of coupling constants, identification of H in various chemical environments to assign structure to the organic molecules using chemical shift values, resonance coupled and decoupled spectra ^{13}C NMR, applications of ^{13}C NMR to find the different carbon functional groups.

UNIT-V: Mass spectra

Mass spectra – theory, principle, instrumentation and applications. McLafferty rearrangement, fragmentation pattern, Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Text Books

1. Y. R. Sharma, Elimentary Organic Spectroscopy, 1st Edn., S. Chand & Company Ltd, New Delhi, 1980.
2. J. Dyer, Application of absorption spectroscopy of organic compounds, Prentice-Hall of India Pvt. Ltd., New Delhi, 2005
2. Raymond Chang, Basic principles of Spectroscopy, McGraw Hill Ltd., New York, 1971
3. C.N. Banwell, Fundamentals of Molecular spectroscopy, McGraw Hill, Newyork, 1966.

Reference Books

1. R.M Silverstein, C.G. Bassler and Monsil, Spectrometric identification of organic compounds, 6th Edn., John Wiley & Sons, New York 2004.
2. William Kemp, Organic Spectroscopy, ELBS, New Delhi, 1982.
3. S. Kalsi, Spectroscopy of organic compounds, 5th Edn., Wiley Eastern Ltd., Madras, 2002.
4. C.N. Banwell, Fundamentals of Molecular Spectroscopy, McGraw Hill, New York,1966.
5. A. Carrigton and A.D. McLachlan, Introduction to Magnetic Resonance, Harper and Row New York 1967.
6. R. Drago, Physical methods in Inorganic Chemistry, Reinhold, Ny.1968.
7. G.M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, NewYork, 1962.
8. W. Kemp, NMR in Chemistry, MacMillan Ltd,1986.
9. G.W. King, Spectroscopy and Molecular structure, Holt, Rienehart and Winston 1964.
10. C.N.R. Rao, J.R. Ferraro, Spectroscopy in Inorganic Chemistry, Methven Co., London. 1968.
11. Raymond Chang, Basic Principles of Spectroscopy**,** Mc Graw Hill Ltd., New York,

109PCHT06: NANOMATERIAL AND GREEN CHEMISTRY

UNIT-I: Introduction to Nanotechnology

Definition, classification, a historical perspective, nanoparticles, nanocrystal, quantum dot, nanometer., new properties of nanomaterials, nanomaterials in medicine, information storage, sensors, new electronic devices, environmental remediation, clean catalysts. Metal nanoparticles, Chemical bonding and properties of bulk metals as well as metal nanoparticals. Gas phase and chemical synthetic methods to metal nanoparticles, nanoelectrons, conductivity of nanoelectrons.

UNIT-II: Properties and Applications of Nanocrystals

Nanotubes, Nanocrystal shape, Sequestration of gases, destructive adsorption of environmental toxins, Optical properties, Magnetic properties of nanoscale materials – diamagnetism, paramagnetism, ferromagnetism, and supermagnetism. Size dependent properties such as coercivity (magnetic memory) and saturation magnetization, nanoparticles in polymers, inks, fluids, dyes and catalysis. Nanocrystals as colorants, ultraviolet absorbers, electronics and in biomedical applications.

UNIT-III: Green Chemistry Basics

The need for green chemistry and eco-efficiency, environmental protection laws, challenges and green chemistry education, pollution control and pollution prevention – green methods, green products, recycling of waste.

Twelve principles of green chemistry, inception of green chemistry, awards for green chemistry and international organizations promoting green chemistry.

UNIT-IV: Solvent Free Organic Synthesis

Solvent free microwave assisted organic synthesis – microwave activation, microwave heating, advantages of microwave exposure and specific effects of microwaves. Organic synthesis under microwaves – benefits, limitations, equipments.

Reactions on solid supports, phase transfer catalysis, solvent free esters saponification, reactions without support or catalyst, examples – microwave assisted reactions in water – oxidation of toluene to benzoic acid, microwave assisted reactions in organic solvent Diels Alder reaction.

UNIT-V: Designing Green Synthesis

Designing Green Synthesis – choice of starting materials, choice of reagents, choice of catalysts – bio catalysts, polymer supported catalysts, choice of solvents.

Synthesis involving basic principles of green chemistry – examples – synthesis of adipic acid, methyl methacrylate, paracetamol.

Ultrasound assisted reactions – esterification, reduction, coupling reactions. Strecker synthesis and reformatsky reaction.

Text Books

1. Kenneth . Klabunde, Nanoscale Materials in Chemistry, John Wiley & Sons, Inc. 2002.
2. Rashmi Sanghi, M. M. Srivastava, Green Chemistry, Environment Friendly Alternatives, Narosa Publishing House, 2007.
3. V. Kumar, An Introduction to Green Chemistry, Vishal Publishing CO. Jalandhar, 2007.

109PCHP01: PRACTICAL- I -ORGANIC CHEMISTRY

I. Identification of components in a two component mixture and preparation of their derivatives. Determination of boiling point/melting point for components and melting point for their derivatives.

II. Preparation

1. Beta naphthyl methl ether from beta naphthol
2. s–Benzyl isothiuronium chloride from benzylchloride
3. Beta glucose penta acetate from glucose
4. ortho- Benzoyl benzoic acid from phthalic anhydride
5. Resacetophenone from resorcinol
6. para- Nitrobenzoic acid from para nitrotoluene
7. meta-Nitroanilline from meta dinitrobenzene
8. Methyl orange from sulphanillic acid
9. Anthraquinone from antracene
10. Benzhydrol from benophenone

Reference: Laboratory Manual of Organic Chemistry – B. B. Dey, M. V. Sitaraman.

109PCHP02: PRACTICAL – II- INORGANIC CHEMISTRY

Part – I

Semimicro qualitative analysis of mixtures containing two common and two rare cations. The following are the care to be included: W, Tl, Mo, Te, Se, Ce, Th, Be, Zr, V, U and Li.

Part – II

a) Colorimetric analysis: visual and photometric; determination of iron, nickel, manganese and copper.
b) Preparation of the following:
    i. Potassium trioxalatoaluminate (III) trihydrate
    ii. Tristhioureacopper (I) chloride
    iii. Potassium trioxalatochromate (III) trihydrate
    iv. Sodium bis (thiosulphato) cuprate (I)
    v. Tetramminecopper (II) sulphate
    vi. Potassium Tetrachlorocuprate (II)
c) Separation of mixture of two metal ions by paper chromatography.

109PCHP03: PRACTICAL – III-- PHYSICAL CHEMISTRY

Experiments in chemical kinetics, phase rule, Chemical equilibrium and Conductivity measurements:

DETAILED LIST OF EXPERIMENTS

Typical list of possible experiments are given. Experiments of similar nature and other experiments may also be given. The list given is only a guideline. A minimum of 15 experiments have to be performed in a year.

1. Study the kinetics of acid hydrolysis of an ester, determination of the temperature coefficient of the reaction and determination of the activation energy of the hydrolysis of ethylacetate.

2. Study the kinetics of the reaction between acetone and iodine in acidic medium by half life method and determine the order with respect to iodine and acetone.

3. Study of the saponification of ethylacetate by sodium hydroxide conductometrically and determine the order of the reaction.

4. Determination of association of ethylacetate by sodium hydroxide conductomertically and determine the order of the reaction.

5. Study the phase diagram for m-toluidine and glycerine system.

6. Construction of phase diagram for a simple binary system (naphthalene-phenanthrene and benzophenone-diphenylamine).

7. Construction of the phase diagram of the three component of partially immiscible liquid systems (DMSO-Water-Benzene; Water-Benzene-Acetic acid; Ethyl alcohol-Benzene-Water; Acetone-Chloroform-Water; Chloroform-Acetic acid-Water).

8. Determination of the equilibrium constant of the reaction between Iodine and KI by partition method.

9. Determination of equivalent conductance of a weak acid at different concentrations and verify Ostwald's dilution law and calculation of the dissociation constant of the acid.

10. Determination of equivalent conductivity of a strong electrolyte at different concentrations and examine the validity of the Onsager's theory as limiting law at high dilutions.

11. Conductometric titrations of a mixture of HCL and CH_3COOH against Sodium hydroxide

12. Compare the relative strength of acetic acid and monochloroacetic acid by conductivity method.

209PCHT01: ORGANIC CHEMISTRY – II

UNIT I Molecular Rearrangements

A detailed study of the mechanism of the following rearrangements: Nucleophilic, Electrophilic and Freeradical rearrangements- memory effects, migratory aptitudes, Pinacol-Pinacolone, Wagner-Meerwin, Demyanov, Dienone-Phenol, Favorski, Baeyer-Villiger, Wolff, Stevens, Von-Richter, Clasien, Hofmann, Schmidt, Lossen, Curtius, Beckmann and Fries rearrangements (a few examples in each rearrangement are to be studied).

UNIT II Reagents in Organic Synthesis

Synthesis of simple organic molecules using standard reactions like acylation and alkylation of enamines and active methylene compounds. Sulphur ylides, Robinson annulation, protection and deprotection of functional groups (R-OH, R-CHO, RCOR, R-NH_2 and R-COOH) Reagents and their uses: DCC, trimethyl silyl iodide, trimethyl silyl chloride, 1,3-dithiane (umpolung), diisobutylaluminium hydride (DIBAL), 9BBN.

UNIT III Oxidation and Reduction Reactions

Study of the following oxidation reactions with mechanism: Oxidation of alcohols by CrO_3, DMSO alone, DMSO in combination with DCC; acetic anhydride and oxalyl chloride, oxidation of arylmethane, oxidation of methylene alpha to carbonyl, allylic oxidation of olefins, oxidative cleavage of glycols, oxidative cleavage of double bonds by ozonolysis.

Study of the following reduction reactions with mechanism: Reduction of carbonyl compounds by hydrides, selectivity in reduction of 4-ter-butyl cyclohexanone using selectrides, Clemmensen and Wolff Kishner reductions, Birch reduction, MPV reduction.

UNIT IV Elimination and Addition Reactions \

Elimination Reactions : E1, E2, E1cB mechanisms, Orientation of the double bond - Hofmann and Saytzeff rule, dehydration and dehydrohaloganation reactions, stereochemistry of E2 eliminations in cyclohexane ring systems, mechanism of pyrolytic eliminations, Chugaev reaction and Cope elimination.

Addition *Reactions :* Addition of halogen and nitrosyl chloride to olefins, hydration of olefins and acetylenes, hydroboration, Michael addition, 1,3 dipolar addition, Diels-Alder

reaction. Mechanism and reactivity. Mannich, Stobbe, Darzen Glycidic ester condensation, Peterson olefination(Silyl Wittig reaction), Strecker synthesis, Perkin , Thorpe , Ritter , Prins reactions.

UNIT V BioOrganic Chemistry

Proteins, polypeptides and their synthesis (upto a tripeptide), solid phase synthesis (Merrifield synthesis), determination of primary structure of proteins (end group assay), discussion on secondary and tertiary structure of proteins.

Structure and role of (genetic code) DNA and RNA.(Determination of structure is not required)

Biosynthesis of amino acids (phenylalanine, tyrosin, 3,4-dopa, praline only) and cholesterol.

Text Books

1. Jerry March, Advanced Organic Chemistry- Reactions, Mechanisms and Structure, Fourth Edition, John Wiley & Sons, 1992.
2. Francis A. Carey, Organic Chemistry, Third Edition, The McGraw-Hill Companies, Inc, 1996.
3. P. S. Kalsi, Organic Reactions and Mechanisms, Second Edition, New Age International Publishers, 2000.
4. I.L. Finar, Organic Chemistry, Volume. II, Fifth Edition, First Indian reprint, Pearson Education Asia Pte. Ltd., 2000.

Reference Books

1. S.H. Pine, J.B. Hendrickson, D.J. Cram and G.S. Hammond, Organic Chemistry, IV Edn. McGraw-Hill Company 1980.
2. S.M. Mukherji and S.P. Singh, Reaction Mechanism in Organic Chemistry, III Edn. 1984, MacMillan.
3. R.T. Morrison and R.N. Boyd, Organic Chemistry, Prentice-Hall, 6^{th} Edn.,1992.
4. R.O.C. Norman, Principles of Organic Synthesis, Second Edition, Chapman and Hall, 1978.
5. Neil Issac, Physical Organic Chemistry, J. Wiley, New York, 1987.
6. Paul de Mayo, Molecular Rearrangements, Vol.I, Vol. II, Interscience, NY, 1963.

209PCHT02: INORGANIC CHEMISTRY-II

UNIT I Boron compounds and Clusters

Boron hydrides - polyhedral boranes, hydroborate ions-a general study of preparation, properties and structure, styx numbers , Wade's rules.

Carboranes - types such as closo and nido-preparation, properties and structure. Metallo carboranes - a general study.

Metal clusters - Chemistry of low molecularity metal clusters only-structure of Re_2Cl_8; multiple metal-metal bonds.

UNIT II Solid - State Chemistry

Structure of Solids; comparison of X-ray, neutron and electron diffractions; Structure of NiAs, CdI_2, Pervoskite, spinels and inverse spinels; defects in solids - point defects, line defects and surface defects; Non-stoichiometric compounds; Use of X-ray powder data in identifying inorganic crystalline solids; details for cubic systems.

Electrical properties of solids - Band Theory, semiconductors, super conductors, solid state electrolytes; Magnetic properties - dia, para, ferro, antiferro and ferrimagnetism; hysterisis; ferrites; garnets; Optical properties – solid - state lasers and Inorganic phosphors.

Reactions in solid state and phase transitions - diffusion coefficient, diffusion mechanism, vacancy and interstitial diffusions, formation of spinels; solid solutions, order-disorder transformations and super structure.

UNIT III Reaction mechanisms in Complexes

Electron transfer reactions - Outer and inner sphere processes; atom transfer reaction, formation and rearrangement of precursor complexes, the bridging ligand, successor complexes; Cross reactions and Marcus-Hush theory; Application of electron transfer reactions in synthesis.

Reaction mechanism of coordination compounds - Substitution reactions, Labile and inert complexes; Kinetic application of V.B and C.F.Theories.

Substitution in square planar complexes - General mechanism; reactivity of Platinum complexes; influences of entering and leaving groups; the trans effect - theories, trans influence.

Substitution in octahedral complexes - general mechanism, discussion of A, D, I_A, I_D and DC_B mechanism; replacement of coordinated water; mechanism of acid hydrolysis and base hydrolysis - Conjugate base mechanism; direct and indirect evidences in favour of the mechanism; application of substitution reaction in the synthesis of Platinum and Cobalt complexes.

UNIT – IV Organometallic Chemistry & Catalysis

Carbon donors - Alkyls and Aryls-preparation and properties; Carbonyls -18 electron rule, isolobal concept - application to structure of carbonyls (simple and polynuclear); Nitrosyls - bridging and terminal nitrosyls, bent and linear nitrosyls; dinitrogen complexes; Chain Carbon donors - Olefins, acetylene and allyl complexes - synthesis, structure and bonding; Cyclic Carbon donors - Metallocene - synthesis, structure and bonding (Ferrocene only).

Reactions - Association reaction - Only ligand protonation; substitution - electrophilic and nucleophilic attack on ligands; addition and elimination; carbonylation and decarbonylation; oxidative addition to organometallics; fluxional isomerism.

Hydrogenation of olefins (Wilkinsons catalyst); hydroformylation of olefins using Cobalt or Rhodium catalysts (oxo process); Oxidation of olefins to aldehydes and ketones (Wacker process); polymerization (Zeigler-Natta catalyst); Cyclo oligomerization of acetylene using Nickel catalyst (Reppe's catalyst); polymer bound catalysts.

UNIT –V Bioinorganic Chemistry

Metal ions in biological systems - essential and trace metals, Na^+/K^+ Pump; Biologically important complexes of Iron (transport proteins) - haemoglobin, myoglobin, iron-sulphur proteins, cytochrome-C, Magnesium (chlorophyll), Cobalt (vitamin B_{12}), Zinc (carbonic anhydrase, carboxy peptidase); macrocyclic effect; fixation of Nitrogen.

Text books

1. J.E. Huheey, E.A. Keiter and R.L. Keiter, **Inorganic Chemistry- Principles of structure and reactivity**, 4th edition, Pearson-Education, 2002.
2. F.A. Cotton and G. Wilkinson, **Advanced Inorganic Chemistry,** Wiley Eastern, 5th edition, 1988.

3. E.A.V. Ebsworth, D.W.H. Rankine and S. Craddock, **Structural methods in Inorganic Chemistry,** Black well Scientific Publ., 1987.
4. R.S. Drago, **Physical Methods in Chemistry,** Reinhold, New York, 1968.
5. Charles A. Depuy and Orville L. Chapman, **Molecular reactions and photochemistry,** Prentice Hall, 1992.
6. A.W. Adamson and P. Fleischauer, **Concepts of Inorganic Photochemistry**, Wiley, 1975.
7. D.A. Skoog and D.M. West, **Fundamentals of Analytical Chemistry**, Holt Rinehart and Winston Publications, IV Edn, 1982.
8. D.A. Skoog, **Principles of Instrumental Analysis**, Saunders College Pub. Co, III Edn., 1985.
9. J.G. Dick, **Analytical Chemistry**, McGraw Hill Publishers, 1974.
10. A.I Vogel, Text Book of Quantitative Inorganic Analysis, Pearson V Edn., 2001.

Reference Books

1. E.L. Mutteri, **Polyhedral boranes**, Acadamic press, NY, 1975.
2. N.H. Ray, **Inorganic polymers**, Academic press, NY, 1975.
3. K.F. Purcell and J.C. Kotz, **Inorganic Chemistry,** WB Saunders Co. USA 1977.
4. G.S. Manku, **Inorganic Chemistry,** TMH Co., 1984.
5. N.J. Turro, **Modern molecular photochemistry**, Benjamin/Cummings, Menlo Park, California, 1978.
6. C.N.R. Rao and J.R. Ferraro**, Spectroscopy in Inorganic Chemistry**, Vol I and Vol II, Academic Press, 1970.
7. H.A.O. Hill and P. Day, **Physical methods in advanced Inorganic Chemistry**, John Wiley, 1986.
8. Willard, Merit, Dean and Settle, **Instrumental Methods of Analysis**, CBS Publishers and Distributors, IV Edn.,1989
9. G. D. Christian and J.E.O Reilly, **Instrumental Analysis**, Allyn and Bacon Inc, II Edn., 1986.
10. G.W. Ewing, **Instrumental Methods of Chemical Analysis**, McGraw Hill Pub, 1975.
11. J.H. Knox (Ed), **High Performance Liquid Chromatography**, Edinburgh University Press, Edinburgh, 1982.

209PCHT03: PHYSICAL CHEMISTRY – II

UNIT – I Quantum Chemistry –I

Photoelectric effect – De Broglie equation – Heisenberg uncertainty principle – Compton effect – operators and commutation relations – quantum mechanical postulates – Schordinger equation and its solution to the problem of a particle in one , three dimensionel boxes and harmonic oscillator. Schrodinger equation for the rigid rotator and Hydrogen atom – arriving solution for energy and wave function – the orgin of quantum numbers and their physical significance – Probability distribution of electrons.

UNIT –II Quantum Chemistry –II

Born – Oppenheimer approximation, Approximation methods – Perturbation and Variation methods – application to Hydrogen and Helium atom – Spin- orbit interaction- LS coupling and JJ coupling- Term symbols and spectroscopic states. Concept of Hybridisation – sp, sp^2 and sp^3 hybridisation , Huckel Molecular orbital (HMO) theory for conjugated π - system , application to simple systems such as Ethylene, butadiene and benzene, Self consistant field approximation – Hartree's and Hartree- Fock Self Consistent field theory, Slater type orbitals – Slater rules.

UNIT-III Electrochemistry –I

Ions in solutions – Debye – Huckel theory of strong electrolytes – Debye-Hückel-onsager equation – verification and limitation – Debye – Hückel limiting law and its extension. Electrode – Electrolyte interface adsorption at electrified interface – electrical double layers – Electro capillary phenomena – Lippmann capillary equation – structure of double layers – Helmholtz Perrin, Guoy Chappman and Stern models of electrical double layers-electro kinetic Phenomena - Tiscelius method of separation of proteins – membrane potential.

UNIT –IV Electrochemistry –II

Mechanism of electrode reactions –the Butler Volmer equation for one step electron transfer reaction – significance of equilibrium exchange current density and symmetry factor – transfer coefficient and its significance – Cyclic voltametry – Principles and applications. Mechanism of Hydrogen and Oxygen evolution reactions. Corrosion and Passivation of metals – construction of Pourbaix and Evans diagrams – Prevention of Corrosion. Electrochemical

energy systems – Primary and Secondary batteries – (dry cells, lead acid – storage batteries, silver - zinc cell, nickel - cadmium battery, mercury cell) – Fuel cells**.**

UNIT –V Surface Chemistry and Catalysis

Kinetics of surface reactions : Physical and chemical adsorption – adsorption isotherms – types of adsorption isotherms – Langmuir adsorption isotherm – B.E.T. theory for multilayer adsorption – application of transition state theory to adsorption – measurement of surface area – Mechanism of heterogeneous catalytic reactions – the adsorption coefficient and its significance.

Acid – Base catalysis – mechanism – Bronsted catalysis Law – catalysis by enzymes – rate of enzyme catalysed reactions – effect of substrate concentration, pH and temperature on enzyme catalysed reactions – inhibition of enzyme catalyzed reactions.

Text Books

1. Gurudeep raj, Advanced Physical chemistry, Goel Publishing House, Meerut.
2. R.K. Prasad, Quantum Chemistry, Wiley Eastern, New Delhi, 1992.
3. M.W. Hanna, Quantum Mechanics in Chemistry, W.A. Benjamin Inc, London 1965.
4. D.A. McQuarrie, Quantum Chemistry, University Science Books, Mill Valley, California, 1983.
5. S. Glasstone, Introduction to Electrochemistry, Affiliated East West press, New Delhi, 1960.
6. D.R. Craw, Principles and Applications of Electrochemistry, Chapman and Hall, 1991.
7. J. Rajaram and J.C. Kuriacose, Kinetics and mechanism of chemical transformation, Macmillan India Ltd., (1993).
8. K.J. Laidlar, Chemical kinetics, Harper and Row, New York (1987).

Reference Books

1. A.K. Chandra, Introductory Quantum Chemistry, Tata McGraw Hill.
2. P.W. Atkins, Molecular Quantum Mechanics, Oxford university press, Oxford, (1983)
3. J,N, Murrell, S.F.A. Kettle and J.M. Tedder, The Chemical Bond, Wiley.
4. J.O.M. Bockris and A.K.N. Reddy, Electrochemistry, Vols 1 and 2, Plenum, New York 1977.
5. C.M.A. Brett and A.M.O. Brett, Electrochemistry, Principles, Methods and application, OUP, Oxford (1993).
6. R.H. Rieger, Electrochemistry, Chapmann and Hall, New York (1994).
7. P. Delahay, Electrode kinetics and structure of Double layer, Interscience, 1965.
8. R.G. Frost and Pearson, Kinetics and Mechanism, Wiley New York (1961).
9. J.W. Moore and R.G. Pearson, Kinetics and Mechanism (1981).
10. C. Capellos and B.H.J. Bielski, Kinetic systems, Willey inter science, New York (1968).
11. G.M. Harris, Chemical Kinetics, D.C. Heath and co, (1966).

209PCHT04: PHOTOCHEMISTRY

UNIT - I Organic Photochemistry

Photochemical reactions: fate of excited molecules, Jablonski diagram, Norrish Type I and Norrish Type II reactions, photoreduction of ketone, photoaddition reactions, Paterno Buchi reaction, di-pi methane rearrangement, photochemistry of arenas, Photooxidation (Formation of peroxy compounds), Photoisomerization (Cis-trans isomerization), Photo addition of olefins and amines to aromatic compounds, Photo rearrangements: Photo-Fries rearrangement and Photo rearrangement of 2,5-Cyclohexadienones.

UNIT –II Inorganic Photochemistry

Photosubstitution, Photoredox, photoisomerisation and photo rearrangementreactions in inorganic complexes. Photovoltaic and Photogalvanic cells – Photoelectrochemical cells – photoassisted electrolysis of water – aspects of solar energy conversion. Application of metal complexes in solar energy conversion

UNIT –III Physical Photochemistry

Absorption and emission of radiation – Franck – Condon principle – decay of electronically excited states, spin allowed and spin forbidden transition. Radiative and non – radiative processes - theory of radiationless transition – Internal conversion and intersystem crossing. Radiative processes - Fluorescence and Phosphorescence – Theory of Fluorescence and Phosphorescence. Factors affecting Fluorescence and Phosphorescence –Prompt and delayed Fluorescence- Fluorescence and structure. quenching of Fluorescence – static and dynamic quenching – Stern – volmer equation

UNIT IV Techniques and application of Photochemistry

Techniques and application of Photochemistry – Quantum yield – Experimental determination of quantum yield – Actinometry – chemical Actinometry - steady state treatment of quantum yield – Resons for high and low quantum yield – life time measurements – radiative and non-radiative life time measurements – Kinetics of Photochemical reaction – Photosensitized reactions.

UNIT V Pericyclic Reactions

Pericyclic reactions, classification, orbital symmetry, Woodward Hofmann rules, selection rules and stereochemistry of electrocyclic reactions, cycloaddition and sigmatropic shifts, analysis by correlation diagram method and Frontier molecular orbital method, Sommelet, Hauser,Cope and Claisen rearrangements.

Text Books

1. Charles H. DePuy, Orville L. Chapman **Molecular Reactions and Photochemistry**, Prentice Hall of India Private Limited, New Delhi, 1988.
2. K.K. Rohatgi Mukherjee, **Fundamentals of Photochemistry**, Wiley Eastern Ltd., 1978.
3. N.J. Turro, **Modern molecular Photochemistry** Benjamin / Cummings, Menlo park, California (1978).
4. A.W. Adamson and P. Fleischauer, **Concepts of Inorganic Photochemistry**, Wiley, 1975.

References

1. J.C.Calvert and J.N.Pitts, **Photochemistry**, Wiley, London 1966.
2. R.P.Wayne, **Photochemistry**, Butterworths, London 1970.
3. R.P.Cundell and A.Gilbert, **Photochemistry**, Thomas Nelson, London, 1970.

209PCHT05: SPECTROSCOPY– II

UNIT I Atomic Absorption Spectroscopy

Atomic absorption spectroscopy – theory, principle, instrumentation. EMR sources – cells, furnaces, detectors; interferences and their corrections; applications of AAS.

UNIT –II ESR Spectroscopy

ESR Spectroscopy: Basic principles, Instrumentation, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants. Applications of ESR spectroscopy. Electronic Zeeman effect – hyperfine interactions – Spin densities – Mcconnel relationship – selection rules in ESR – bonding parameters from 'g' and coupling constants.

UNIT –III Mossbauer Spectroscopy

Mossbauer Spectroscopy - Doppler effect; isomer effect; electron-neutron hyperfine interactions; Quadrupole interactions and magnetic interactions; simple applications to Iron and Tin compounds.

UNIT –IV Photoelectron Spectroscopy

Photoelectron Spectroscopy - Principle, PES of diatomic molecules and polyatomic molecules (HCl, HBr, HI, CO, NH_3, H_2O and N_3^- ion); Core electron PES; X-ray photoelectron spectroscopy (ESCA) applications.

UNIT –V ORD-CD

ORD-CD : Definition, circular birefringence and circular dichroism, plain dispersion curves and their applications, single and multiple cotton effect curves, structural and stereochemical applications – axial haloketone rule, octant rule for ketones, Comparison of ORD and CD.

Text Books

1. D.A. Skoog and D.M. West, Fundamentals of Analytical Chemistry, Holt Rinehart and Winston Publications, IV Edn, 1982.
2. D.A. Skoog, Principles of Instrumental Analysis, Saunders College Pub..Co., III Edn., 1985.
3. J.G. Dick, Analytical Chemistry, McGraw Hill Publishers, 1974.
4. C.N.R. Rao and J.R. Ferraro, Spectroscopy in Inorganic Chemistry, Vol I and Vol II, Academic Press, 1970.
5. H.A.O. Hill and P. Day, Physical methods in advanced Inorganic Chemistry, John Wiley, 1986.
6. Willard, Merit, Dean and Settle, Instrumental Methods of Analysis, CBS Publishers and Distributors, IV Edn.,1989
7. G. D. Christian and J.E.O Reilly, Instrumental Analysis, Allyn and Bacon Inc, II Edn., 1986.
8. G.W. Ewing, Instrumental Methods of Chemical Analysis, McGraw Hill Pub., 1975.
9. R.S. Drago, Physical Methods in Chemistry, Reinhold, New York, 1968.
10. C. Djerassi, Optical rotatory dispersion- application to organic chemistry, McGraw Hill, 1960.

209PCHT06: ENVIRONMENTAL CHEMISTRY

UNIT - I COMPOSITION

Composition of atmosphere, vertical temperature, heat budget of the earth atmospheric system, vertical stability atmosphere, biogeochemical cycles of C, N, P, S and O. Biodistribution of elements. Soil composition, micro and macro nutrients, pollution – fertilizers, , pesticides, plastics and metals. Waste treatment.

UNIT - II HYDROSPHERE

Aquatic pollution – inorganic, organic, pesticides, agricultural, industrial and sewage, detergents, oil spills and oil pollutants. Water quality parameters – dissolved oxygen, biochemical oxygen demand, solids, metals, content of chloride, sulphate, phosphate, nitrate and micro organisms, water quality standards.

UNIT - III ATMOSPHERE

Chemical composition of atmosphere – particles, ions and radicals and their formation, chemical and photochemical reactions in atmosphere, smog formation, oxides of N, C, S, O and their effect, pollution by chemicals, petroleum, minerals, chlorofluoro hydrocarbons. Air pollution control and their chemistry.

UNIT - IV INDUSTRIAL POLLUTION

Cement, sugar, distillery, drug, paper and pulp, thermal power plants, nuclear power plants, metallurgy, polymers and drugs. Radionuclide analysis, Disposal of wastes and their management.

UNIT - V ENVIRONMENTAL TOXICOLOGY

Chemical solutions to environmental problems, biodegradability, principles of decomposition, better industrial processes. Bhopal gas tragety, Chernobyl, Three miles island, Sewozo and Minamata disasters.

TEXT BOOKS

1. Ed.J. Rose, Environmental Toxicology, Gordon and Breach Science Publication.
2. Ed.S. Landsberger and M. Creatchman, Elemental Analysis of Airborne Particles, Gordon and Breach Science Publication.
3. S.E. Manahan, Environmental Chemistry Lewis Publishers.
4. Sharma & Kaur, Environmental Chemistry Krishna Publishers.
5. A.K.DE., Environmental Chemistry, Wiley Eastern.
6. S.M. Khopkar, Environmental Pollution Analysis, Wiley Eastern.

209PCHP01: PRACTICAL – IV-- ORGANIC CHEMISTRY - II

I. Organic Estimation

1. Phenol
2. Aniline
3. Methyl Ketone
4. Glucose
5. Iodine value of an oil
6. Saponification value of an oil.

II Organic Preparation, Involving Two Stages

1. Sym-tribromobenzene from aniline.
2. m-Nitrobenzoic acid from methyl benzoate
3. para -Nitroaniline from acetanilide.
4. Benzanilide from benzophenone.
5. para –Amino benzene sulphanamide from acetanilide
6. Anthraquinone from phthalic anhydride.

III. Extraction of Natural Products:

1. Caffeine from tea leaves.
2. Citric acid from lemon.

IV Chromatographic Separations

1. Column chromatography : separation of a mixture of ortho and para-Nitroanilines.
2. Thin layer Chromatography : separation of a mixture of ortho and para – Nitroanilines.
3. Paper chromatography – identification of natural alpha amino acids.

Ref : 1. Vogel's Practical organic chemistry.
2. Laboratory manual of organic chemistry – B.B. Dey and M.V. Sitaraman.

209PCHP02: PRACTICAL -V-- INORGANIC CHEMISTRY - II

Part I Quantitative analysis of complex materials

A) Quantitative analysis :
Quantitative analysis of mixture of iron and magnesium; iron and nickel, copper and nickel and copper and zinc.

B) Analysis of Ores

1. Determination of percentage of calcium and magnesium in dolomite.
2. Determination of percentage of MnO_2 in pyrolusite
3. Determination of percentage of lead in galena.

C) Analysis of Alloys

1. Determination of tin and lead in solder.
2. Determination of copper and zinc in brass.
3. Determination of Chromium and nickel in stainless steel.

Part II : Preparations of the following :

1. Sodium hexanitrocobaltate (III)
2. Tris (ethyleneamine) Cobalt (III) chloride
3. Chloropentammine Cobalt (III) chloride
4. Bis (acetylacetanato) Copper (II)
5. Hexamminecobalt (III) chloride
6. Hexamminenickel (II) chloride.

Reference Books for Inorganic Chemistry Practicals I and II

1. Vogel's **Qualitative Inorganic analysis** Revised by G.Svehla, VI Edition, orient Longmax (1987).
2. V.V. Ramanujam, **Inorganic Semimicro Qualitative analysis**, National Publishing co. 1971.
3. J. Basset, R.C. Denney, G.H. Jeffery and J. Mendham Vogel's **Text book of quantitative inorganic analysis,** ELBS, IV Edition(1985).
4. W.G. Palmer, **Experimental Inorganic Chemistry**, Van Nostrand Reinhold Co., London 1972.
4. D.N. Grindley, **An advanced course in practical Inorganic Chemistry**, Butterworths 1964.

209PCHP03: PRACTICAL – VI-- PHYSICAL CHEMISTRY - II

Experiments in electro chemistry, Polarography and Chemical Kinetics.

EMF Measurements

Determination of standard potentials (Cu and Ag)

Determination in thermodynamic quantities from EMF measurements, Potentiometric titrations

Determination of p_H and calculation of $p^K_{a.}$

Determination of stability constant of complex.

Determination of solubility product of a sparingly soluble salt, Redox titrations.

Precipitation titration of mixture of halides by emf measurements.

DETAILED LIST OF EXPERIMENTS

Typical list of possible experiments are given. Experiments of similar nature and other experiments may also be given. The list given is only a guideline. A minimum of 15 experiments have to be performed.

1. Determination of the activity coefficient of an electrolyte at different molalities by emf measurements.

2. Determination of the dissociation constant of acetic acid by titrating it with sodium hydroxide using quinhydrone as an indicator electrode and calomel as a reference electrode.

3. Determination of the strength of a given solution of KCl using differential potentiometric titration technique.

4. Determination of the P^H of the given solutions with the help of the indicators using buffer solutions and by colorimetric method.

5. Determination of the P^H of a given solution by emf method using hydrogen electrode and quinhydrone electrode.

6. Determination of the composition and instability constant of a complex by mole ratio method.

7. Calculation of the thermodynamic parameters for the reaction $Zn + H_2SO_4 \longrightarrow ZnSO_4 + H_2$ by emf method.

8. Determination of the formation constant of silver ammonia complex and stoichiometry of the complex potentiometrically.

9. Solubility and Solubility products by emf method.

10. Determination of the activity coefficient of Zinc ions in the solution of 0.002 M Zinc sulphate using Debye – Huckel Limiting law.

11. Determination of solubility product of Silver bromide and calculate its solubility in water and 0.01 M and 0.01 M $KbrO_3$ using Debye – Huckel limiting law.

12. Determinations of the electrode potentials of Zn and Ag electrodes in 0.1 M and 0.001 M solutions at 298 K and find the standard potentials for these electrodes and test the validity of Nernst equations.

13. Study the inversion of cane sugar in presence of acid using polarimeter.

14. Determination of the rate constant and order of reaction between potassium persulphate and potassium iodide and determine the temperature coefficient and energy of activation of the reaction.

15. Study the primary salt effect on the kinetics of ionic reactions and test the Bronsted relationship (iodine ion is oxidized by persulphate ion).

16. Determination of the viscosities of mixtures of different compositions of liquids and find the composition of a given mixture.

17. Determination of the partial molar volume of the glycine/methanol/formic acid/sulphuric acid by graphical method and by determining the densities of the solutions of different comparisons.

18. Study the surface tension – concentration relationship for solutions (Gibb's equation).