SOPHIA COLLEGE (AUTONOMOUS)

Affiliated to the University of Mumbai

Programme: **SCIENCE**

Programee code: SCHE

Syllabus for the Academic Year 2023-2024

based on the National Education Policy 2020

(Choice Based Credit System with effect from 2023-2024)

SOPHIA COLLEGE (AUTONOMOUS)

Preamble

Programme: MSc-Analytical Chemistry

The M.Sc. Programme in Analytical chemistry was started under the affiliation of Mumbai University and is now brought under Autonomy. Although the same syllabus has been retained with minor modifications structural changes are incorporated to suit the credit system under autonomy.

The objective of the M.Sc. Analytical Chemistry programme is to provide a comprehensive and in-depth understanding of the fascinating world of Analytical Chemistry. The M.Sc. Programme in Analytical Chemistry combines core and elective theory courses as well as practical courses and independent research guided by an experienced researcher from the department/industry or a national institute. Through a rigorous academic curriculum, industry training and hands-on research experience, we aim to nurture the intellectual curiosity and scientific acumen of our students, preparing them for successful careers in various sectors of the chemical sciences. On completing the programme, the students will be able to analyze and provide practical solutions to the problems within the broad/specialized field of analytical chemistry.

Our esteemed faculty members with expertise in their respective fields and with a passion for both teaching and research are committed to providing a learning environment, encouraging open discussions, and fostering collaborative research endeavors. Through their mentorship, students will have the opportunity to engage in cutting-edge research projects, pushing the boundaries of scientific knowledge and contributing to the advancement of the chemical sciences. We envision our M.Sc. (Analytical Chemistry) postgraduates act as catalysts for positive change, equipped to drive innovation, shape industries, and address societal challenges through their expertise in chemistry.

PROGRAMME OBJECTIVES	
PO 1	To provide students with theoretical and applied knowledge in the interdisciplinary branches of chemistry with emphasis on qualitative and quantitative analysis.
PO 2	To expose the students to the advanced instrumental analysis through hands on training, internships and research to make them job ready.
PO 3	To train students to address the environmental and societal issues and face the real life challenges more effectively.

PROGRAMME SPECIFIC OUTCOMES	
PSO 1	**Critical thinking:** A student with a Master's degree in Analytical chemistry will have an in-depth theoretical and practical knowledge of the subject which will foster their critical thinking.
PSO 2	**Skills in research and industrial field:** Students will build a scientific temper through research, develop entrepreneurial skill and will get an exposure to work in an industrial set up.
PSO 3	**Personality Development:** The students will be able to handle personal, social, environmental issues and will be responsible citizens.

Programee Outline: M.Sc Part 1 (SEMESTER I)

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Course code	Unit no	Name of the unit	Credits

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SCHE511MJ		PHYSICAL AND INORGANIC CHEMISTRY	4
	1	THERMODYNAMICS	
	2	2.1 CHEMICAL KINETICS, MOLECULAR REACTION DYNAMIC 2.2 SOLID STATE CHEMISTRY AND PHASE EQUILIBRIUM	
	3	CHEMICAL BONDING, MOLECULAR SYMMETRY & GROUP THEORY	
	4	COORDINATION COMPOUNDS: SPECTRAL AND MAGNETIC PROPERTIES	
SCHE511PMJ		PRACTICAL	2
SCHE512MJ		ORGANIC AND ANALYTICAL CHEMISTRY	4
	1	PHYSICAL ORGANIC CHEMISTRY,AROMATICITY AND OXIDATION REDUCTION REAGENTS	
	2	STEREOCHEMISTRY	
	3	LANGUAGE AND QUALITY OF/IN ANALYTICAL CHEMISTRY	
	4	CALCULATIONS BASED ON CHEMICAL PRINCIPLES	
SCHE512PMJ		PRACTICALS	2
SCHE511E		ADVANCED INSTRUMENTAL TECHNIQUE	2
	1	OPTICAL METHOD	
	2	SPECTROSCOPY AND RADIO ANALYTICAL METHODS	
SCHE511EP		PRACTICAL	2

SCHE511RM	1	SCIENTIFIC INVESTIGATION	4
	2	DATA REPRESENTATION AND INTERPRETATION	
	3	LABORATORY SAFETY & ETHICAL HANDLING OF CHEMICALS	
	4	LOGICAL MATHEMATICAL REASONING & COMPUTATIONAL TOOLS	

Programee Outline: M.Sc Part I (SEMESTER II)

Course code	Unit no	Name of the unit	Credits
SCHE523MJ		PHYSICAL AND INORGANIC CHEMISTRY	4
	1	QUANTUM CHEMISTRY	
	2	ELECTROCHEMISTRY	
	3	INORGANIC REACTION MECHANISM	
	4	INORGANIC REACTION MECHANISM	
SCHE523PMJ		PRACTICAL	2
SCHE524MJ		ORGANIC AND ANALYTICAL CHEMISTRY	4
	1	1.1REACTIONS AND REARRANGEMENTS 1.2MOLECULAR ORBITAL THEORY	
	2	SPECTROSCOPY	
	3	THERMAL METHODS	
	4	ELECTROANALYTICAL METHODS	
SCHE524PMJ		PRACTICAL	2
SCHE522E		ADVANCED INSTRUMENTAL TECHNIQUE	2
	1	SURFACE ANALYTICAL TECHNIQUES	
	2	CHROMATOGRAPHY	
SCHE22EP		PRACTICAL	2
		ON JOB TRAINING (OJT)	4

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SEMESTER I

NAME OF THE COURSE	PHYSICAL AND INORGANIC CHEMISTRY	
CLASS	M.Sc Part 1	
COURSE CODE	**SCHE511MJ**	
NUMBER OF CREDITS	4	
NUMBER OF LECTURES PER WEEK	4	
TOTAL NUMBER OF LECTURES PER SEMESTER	60	
EVALUATION METHOD	CONTINUOUS ASSESSMENT	SUMMATIVE ASSESSMENT
TOTAL MARKS	50	50
PASSING MARKS	20	20

Course Objectives

CO1	To understand and elucidate the third law of thermodynamics and properties like absolute entropies, heat capacity, entropies of vaporization of liquids etc.
CO2	To learn kinetics of enzyme catalyzed reactions, different types of inhibitions of enzymes and kinetics of reactions in solid state.
CO3	To understand different types and thermodynamics of formation of defects To summarize phase equilibria for two component and three component systems.
CO4	To summarize phase equilibria for two component and three component systems.
CO5	To understand wave functions for different hybridizations and bonding in diatomic and polyatomic species.
CO6	To understand construction of character tables for different point groups and applications of group theory.
CO7	To understand the methods of preparation and properties of co-ordination compounds.
CO8	To understand spectral calculations and magnetic properties of co-ordination compounds.

Course Outcomes: The learner will be able to

CLO1	discuss and elucidate the Third law of thermodynamics, Trouton's rule
CLO2	solve problems using the properties and relationships of thermodynamic fluids
CLO3	elaborate the general mechanisms of acid-base catalysis, enzyme catalysis and effect of pH & temperature on them.
CLO4	extrapolate mathematical equations to find concentration of defects and solve numerical problems based on it.

CLO5	understand and explain two component systems and three component systems.
CLO6	derive wavefunction from different hybridization and plot MOT diagram for diatomic and polyatomic species.
CLO7	Construct character table for different point group and apply of group theory to inorganic molecules.
CLO8	Write the method of preparation and explain the properties of co-ordination compound.
CLO9	Interpret the spectral and the magnetic properties of co-ordination compound.

UNIT I	**THERMODYNAMICS**	**15L**
1.1	State function and exact differentials, Joule Thomson experiment, Joule Thomson coefficient, inversion temperature, Joule Thomson coefficient in terms of Van der Waals constants	
1.2	Third law of Thermodynamics, Entropy change for a phase transition, absolute entropies, determination of absolute entropies in terms of heat capacity, standard molar entropies and their dependence on molecular mass and molecular structure, residual entropy.	
1.3	Entropies of vaporization of liquids – Trouton's rule , Validity, deviation and application, Hildebrand's rule [Ref 2 and 1,10,11,12 17]	
UNIT II	**CHEMICAL KINETICS, MOLECULAR REACTION DYNAMICS , SOLID STATE CHEMISTRY AND PHASE EQUILIBRIUM**	**15L**
	2.1 Chemical Kinetics, Molecular Reaction Dynamics	
	2.1.1 General Catalytic Mechanisms – Equilibrium treatment, steady state treatment, Activation energies for catalyzed reactions Acid base Catalysis – general, theory and mechanism 2.1.2 Kinetics of reactions in the Solid State:-Factors affecting reactions in solids Rate laws for reactions in solid: The parabolic rate law, The first order rate Law, the contracting sphere rate law, Contracting area rate law, some examples of kinetic studies. (Ref: 7 and 2)	

	2.2 Solid State Chemistry and Phase equilibria	
	2.2.1 Types of Defects and Stoichiometry, Zero dimensional (point) Defects, One dimensional (line) Defects, Two dimensional (Planar) Defects Thermodynamics of formation of defects (Mathematical derivation to find concentration of defects and numerical problems based on it) (Ref: 17, 18 and19) 2.2.2 A] Two component system: I. Solid –Gas System : Hydrate formation, Amino compound formation II. Solid – Liquid System: Formation of a compound with congruent melting point, Formation of a compound with incongruent melting point (with suitable examples) B] Three component system: I. Formation of two pair of partially miscible II. Formation of three pair of partially miscible liquid. III. Solid liquid Equilibria - Ternary solutions with common ions – (NaCl – KCl-H_2O and NaCl- Na_4SO_4- H_2O) (Ref: 4, 6, 11, 12 ,13,16, 24)	
UNIT III	**CHEMICAL BONDING, MOLECULAR SYMMETRY & GROUP THEORY**	**15L**
3.1	**Chemical Bonding** **Valence Bond Theory** Recapitulation of hybridization, Derivation of wave functions for *sp*, sp^2, *sp3* orbital hybridization types considering only sigma bonding, and Critical analysis of VBT. Bent's rule:Structure and reactivity of compounds/ complexes **Molecular Orbital Theory:** Molecular Orbital Theory (considering σ bonding) for - diatomic species of the first transition series -polyatomic species: electron deficient (B_2H_6) and electron rich (I_3) molecular species.	
3.2	Symmetry criterion of optical activity, symmetry restrictions on dipole moment, elements of symmetry, A systematic procedure for symmetry classification of molecules.	
3.3	Concepts of Groups, Sub-groups, Classes of Symmetry operations, Group Multiplication Tables. Abelian and non-Abelian point groups. Representation of Groups: Matrix representation of symmetry operations,	

	reducible and irreducible representations. The Great Orthogonality Theorem and its application in construction of character tables for point groups C_{2v}, C_{3v} and D_{2h}, structure of character tables.	
3.4	Applications of Group Theory (a) Symmetry adapted linear combinations (SALC), symmetry aspects of MOT, sigma bonding in AB_n(Ammonia, CH_4) molecule. (b) Determination of symmetry species for translations and rotations. (c) Mulliken's notations for irreducible representations. (d) Reduction of reducible representations using reduction formula. (e)Group subgroup relationships. Applications of Group Theory (a) Symmetry adapted linear combinations (SALC), symmetry aspects of MOT, sigma bonding in AB_n(Ammonia, CH_4) molecule. (b) Determination of symmetry species for translations and rotations. (c) Mulliken's notations for irreducible representations. (d) Reduction of reducible representations using reduction formula. (e)Group subgroup relationships between different groups.	
UNIT IV	**COORDINATION COMPOUNDS: SPECTRAL AND MAGNETIC PROPERTIES**	**15L**
4.1	Methods of preparation, thermal studies, Conductivity measurements, electronic, spectral and magnetic measurements, IR, NMR and ESR spectroscopic methods of characterisation.	
4.2	Spectral calculations using Orgel and Tanabe-Sugano diagrams, calculation of electronic parameters such as Δ, B, C, Nephelauxetic ratio.	
4.3	Magnetic Properties of Coordination Complexes: Origin of magnetism, types of magnetism, Curie law, Curie-Weiss Law, 1st and 2nd Ordered Zeeman effect, quenching of orbital angular momentum by ligand fields, magnetic properties of A, E and T ground terms in complexes, spin free and spin paired equilibria, temperature dependence of magnetism	

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K.J. Laidler and J.H. Meiser, Physical Chemistry, 2nd Ed., CBS Publishers and Distributors, New Delhi, 1999.

Robert J. Silby and Robert A. Alberty, Physical Chemistry, 3rd Edition, John Wiley and Sons (Asia) Pte. Ltd., 2002.

Ira R. Levine, Physical Chemistry, 5th Edition, Tata McGraw-Hill New Delhi, 2002.

G.W. Castellan, Physical Chemistry, 3rd Edition, Narosa Publishing House, New Delhi, 1983.

S. Glasstone, Textbook of Physical Chemistry, 2ndEdition., McMillan and Co. Ltd., London, 1962

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W.G. Davis, Introduction to Chemical Thermodynamics – A Non – Calculus Approach, Saunders, Philadelphia, 19772.

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Thomas Engel and Philip Reid, Physical Chemistry, 3rd Edition, Pearson Education Limited 2013.

D.N. Bajpai, Advanced Physical Chemistry, S. Chand 1st Edition, 1992.

Bockris, John O'M., Reddy, Amulya K.N., Gamboa-Aldeco, Maria E., Modern Electrochemistry, 2A, Plenum Publishers, 1998.

Physical Chemistry by Gurtu and Gurtu

A Textbook of Physical Chemistry by K L kapoorVol 5, 2ndEdition

UNIT 3

CHEMICAL BONDING

B. R. Puri, L. R. Sharma and K. C. Kalia, Principles of Inorganic Chemistry, Milestone Publishers, 2013-2014.

B. W. Pfennig, Principles of Inorganic Chemistry, Wiley, 2015.

C. E. Housecroft and A. G. Sharpe, Inorganic Chemistry, Pearson Education Limited, 2nd Edition 2005.

J. Huheey, F. A. Keiter and R. I. Keiter, Inorganic Chemistry–Principles of Structure and Reactivity, 4th Ed., Harper Collins, 1993.

P. J. Durrant and B. Durrant, Introduction to Advanced Inorganic Chemistry, Oxford University Press, 1967.

R. L. Dekock and H.B.Gray, Chemical Structure and Bonding, The Benjamin Cummings Publishing Company, 1989.

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MOLECULAR SYMMETRY & GROUP THEORY

F. A. Cotton, Chemical Applications of Group Theory, 2nd Edition, Wiley Eastern Ltd., 1989.

H. H. Jaffe and M. Orchin, Symmetry in Chemistry, John Wiley & Sons, New York, 1996.

R. L. Carter, Molecular Symmetry and Group Theory, John Wiley & Sons, New York, 1998.

K. V. Reddy. Symmetry and Spectroscopy of Molecules, 2nd Edition, New Age International Publishers, New Delhi, 2009.

A. Salahuddin Kunju and G. Krishnan, Group Theory and its Applications in Chemistry, PHI Learning, 2012.

P. K. Bhattacharya, Group Theory and its Chemical Applications, Himalaya Publishing House. 2014.

UNIT 4

J. E. Huheey, E. A. Keiter and R. L. Keiter; Inorganic Chemistry: Principles of Structure and Reactivity, Pearson Education, 2006.

D. Banerjea ,Coordination Chemistry

Geary Coordination reviews

P.W. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong; Shriver & Atkins: Inorganic Chemistry, 4th ed. Oxford University Press, 2006.

F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann; Advanced Inorganic Chemistry, 6th ed. Wiley, 1999,

B. Douglas, D. McDaniel and J. Alexander. Concepts and Models of Inorganic Chemistry (3rd Edition.), John Wiley & Sons (1994).

PRACTICALS

NAMEO
PHYSIC

SOPHIA COLLEGE (AUTONOMOUS)

FTHECOURSE	ALANDINORGANICCHEMISTRY
CLASS	M.ScPART1
COURSECODE	SCHE511PMJ
NUMBEROFCRE	2

DITS	
NUMBEROFLECTURESPERWEEK	4
TOTALNUMBEROFLECTURESPE	60

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RSEMESTER	
EVALUATIONMETHOD TOTALMARKS PASSINGMARKS	SUMMATIVEASSESSMENT 50 20

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Learning Objectives:

CO1	To train the students in handling various instruments, glassware, chemicals etc. used in various analyses
CO2	To instruct the learner in practical knowledge on planning and performing experiments.
CO3	To elucidate knowledge about the non-instrumental techniques
CO4	To use classical methods to estimate percentage of metal in alloys/ores
CO5	To use instrumental methods of analysis for estimation of metal ions and inorganic compounds

Learning Outcomes : The learner will be able to

CLO1	carefully handle and use various instruments used in the lab for performing experiments
CLO2	follow instructions thoroughly
CLO3	perform experiments with accuracy and perfection
CLO4	Identify and use simple classical methods and calculate percentage composition of metals in alloys/ores
CLO5	Estimate metal ions and inorganic compounds using instrumental methods

Non – Instrumental:

1. Determine the heat of solution (ΔH) of a sparingly soluble acid (benzoic /salicylic acid) from solubility measurement at three different temperatures.
2. Study the variation of calcium sulphate with ionic strength and hence determine the thermodynamic solubility product of $CaSO_4$ at room temperature.

Instrumental:

1. Verify Ostwald's dilution law and to determine the dissociation constant of a weak mono-basic acid conductometrically.
2. Determine the stability constant of the complex formed between Fe^{3+} ion and 5-sulphosalicylic acid at pH 2 and pH 3 by spectrophotometric method.

I] Analysis of Ores and Alloys/ preparation of compounds

1) Analysis of Devarda's alloy

2) Analysis of Cu – Ni alloy

3) Analysis of Solder alloy

4) Analysis of Limestone.

5) Analysis of hematite ore.

II] Instrumentation:

1) Estimation of Copper using Iodometric method Potentiometrically.

2) Estimation of boric acid conductometrically

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2. The Synthesis and Characterization of Inorganic Compounds by William L. Jolly
3. Inorganic Chemistry Practical Under UGC Syllabus for M.Sc. in all India Universities By:Dr Deepak Pant
4. Practical Physical Chemistry, B. Viswanathan and P.S. Raghavan, Viva Books Private Limited, 2005.
5. Practical Physical Chemistry, A.M. James and F.E. Prichard, 3rd Edition, Longman Group Ltd., 1974.
6. Experimental Physical Chemistry, V.D. Athawale and P. Mathur, New Age International Publishers, 2001

NAME OF THE COURSE	**ORGANIC AND ANALYTICAL CHEMISTRY**	
CLASS	M.Sc Part 1	
COURSE CODE	SCHE512MJ	
NUMBER OF CREDITS	4	
NUMBER OF LECTURES PER WEEK	4	
TOTAL NUMBER OF LECTURES PER SEMESTER	60	
EVALUATION METHOD	CONTINUOUS ASSESSMENT	SUMMATIVE ASSESSMENT
TOTAL MARKS PASSING MARKS	50 20	50 20

Course Objectives

CO1	Understand the criteria of aromaticity, thermochemical and magnetic criteria for aromatic compounds of benzenoid and non-benzenoid structures.

CO2	Learn to draw the Frost Musulin Diagrams for various compounds.
CO3	Understand the stereochemical concepts in molecules with constitutionally symmetric and asymmetric stereoisomers.
CO4	Understand the principles of axial and planar chirality.
CO5	Understand the configurational descriptors to allenes, alkylidene cycloalkanes, spirans, biaryls (including BINOLs and BINAPs), ansa compounds, cyclophanes,
CO6	Understand the concepts of topicity, criteria for enantiotopic and disastereotopic ligands and faces and identify them in a stereoisomer.
CO7	Understand how to assign configurational descriptors for enantiotopic and diastereotopic faces
CO8	Understand the concept of prochirality and predicting them in a molecule
CO9	To introduce important terms involved in analytical chemistry
CO10	To create awareness about quality, accreditation and GLP
CO11	To learn and use appropriate concentration units and predict yield of a reaction.

COURSE OUTCOMES:The learner will be able to

CLO1	Classify the compounds based on criteria of aromaticity, analyse the thermochemical and magnetic data for aromatic compounds of benzenoid and non-benzenoid structures
CLO2	Predicting the aromaticity in cyclic compounds based on Frost Musulin diagram
CLO3	Predicting the stereochemical concepts in molecules with constitutionally symmetric and asymmetric stereoisomers.
CLO4	Applying the principles of axial and planar chirality.
CLO5	Assigning configurational descriptors to allenes, alkylidene cycloalkanes, spirans, biaryls (including BINOLs and BINAPs), ansa compounds, cyclophanes,
CLO6	Predicting topicity, evaluating the criteria for enantiotopic and disastereotopic ligands and faces and identifying them in a stereoisomer and assigning configurational descriptors
CLO7	Identifying a prochiral center in a given molecule and assign the configurational descriptors.
CLO8	Predicting Selectivity and specificity of the various oxidizing and reducing reagents and the mechanisms
CLO9	understand the use and importance of various terms used in analytical chemistry.

CLO10	various quality standards and safety rules followed in the laboratories.
CLO11	interconvert various concentration units and assess conditions to improve reaction yield.

UNIT 1	PHYSICAL ORGANIC CHEMISTRY, AROMATICITY AND OXIDATION REDUCTION REAGENTS	15L
1.1	Thermodynamic and kinetic requirements of a reaction: rate and equilibrium constants, reaction coordinate diagram, transition state (activated complex), nature of activated complex, Hammond postulate, Reactivity vs selectivity, Curtin-Hammett Principle, Microscopic reversibility, Kinetic vs thermodynamic control of organic reactions.	
1.2	Ester hydrolysis: Classification, nomenclature and study of all eight mechanisms of acid and base catalyzed hydrolysis with suitable examples.	
1.3	Aromaticity: Structural, thermochemical, and magnetic criteria for aromaticity, including NMR characteristics of aromatic systems. Delocalization and aromaticity. Application of HMO theory to monocyclic conjugated systems. Frost-Musulin diagrams. Huckel's (4n+2) and 4n rules. Aromatic and antiaromatic compounds up-to 18 carbon atoms. Homoaromatic compounds. Aromaticity of all benzenoid systems, heterocycles, metallocenes, azulenes, annulenes, aromatic ions and Fullerene (C60). [Reference Books 1,2 ,13,16]	
1.4	Oxidation: General mechanism and selectivity of hydrocarbons, alcohols, carbonyl compounds Oxidation of hydrocarbons: Dehydrogenation:(chloranil, DDQ). Oxidation involving C-C bonds cleavage: aromatic rings using RuO4 and NaIO4. Oxidation involving replacement of hydrogen by oxygen: oxidation of CH2 to CO by SeO2, oxidation of aryl methanes by CrO2Cl2 (Etard oxidation). Oxidation of alcohols: CrO3-pyridine (Collin's reagent), hypervalent iodine reagents (IBX, Dess-Martin periodinane). DMSO based reagents (Swern oxidation), Oxidation of aldehydes and ketones: with H2O2 (Dakin reaction), with peroxy acid (Baeyer-Villiger oxidation)	
1.5	Reduction: General mechanism, selectivity, and important applications of the following reducing reagents: Catalytic reduction: Adams Catalyst, Reduction by hydride: diborane, 9-BBN, DIBAL-H, Red Al, Dissolving metal reductions: mediated reduction (Birch reduction) of aromatic compounds and acetylenes. Other Methods of reduction:NH_2NH_2 (diimide reduction) and other non-metal based agents including organic reducing agents (Hantzsch Dihydropyridine).	
UNIT II	**STEREOCHEMISTRY**	**15L**
2.1	Constitutionally symmetrical molecules with odd and even number of chiral centers: enantiomeric and meso forms, concept of stereogenic, chirotopic, and	

	pseudo asymmetric centres.	
2.2	**Axial and planar chirality:** Principles of axial and planar chirality. Recapitulation of : allenes, alkylidene cycloalkanes, spirans, biaryls. Stereochemical features and configurational descriptors (R, S) for the following classes of compounds: allenes, alkylidene cycloalkanes, spirans, biaryls (buttressing effect) (including BINOLs and BINAPs), ansa compounds, cyclophanes.	
2.3	**Prochirality:** Chiral and prochiral centres; prochiral axis and prochiral plane. Homotopic, heterotopic (enantiotopic and diastereotopic) ligands and faces. Identification using substitution and symmetry criteria. Nomenclature of stereo heterotopic ligands and faces Symbols for stereo heterotopic ligands in molecules with i) one or more prochiral centres ii) a chiral as well as a prochiral centre, iii) a prochiral axis iv) a prochiral plane v)pro-pseudo asymmetric centre. Symbols for enantiotopic and diastereotopic faces.	
UNIT III	**LANGUAGE AND QUALITY OF/IN ANALYTICAL CHEMISTRY**	**15L**
3.1	**Language of Analytical Chemistry** **3.1.1** Analytical perspective, Common analytical problems, terms involved in analytical chemistry (analysis, determination, measurement, techniques, methods, procedures and protocol) **3.1.2.** An overview of analytical methods, types of instrumental methods, instruments for analysis, data domains, electrical and non-electrical domains, detectors, transducers and sensors, selection of an analytical method, accuracy, precision, selectivity, sensitivity, detection limit and dynamic range. **3.1.3.** Errors, determinate and indeterminate errors. Types of determinate errors, tackling of errors **3.1.4.** Quantitative methods of analysis: calibration curve, standard addition and internal standard method.	
3.2	**Quality in Analytical Chemistry:** **3.2.1 Quality Management System (QMS)**Evolution and significance of Quality Management, types of quality standards for laboratories, total quality management (TQM), philosophy implementation of TQM (reference of Kaizen, Six Sigma approach & 5S), quality audits and quality reviews, responsibility of laboratory staff for quality and problems. 3.2.2 **Safety in Laboratories:** Basic concepts of Safety in Laboratories, Personal Protection Equipment (PPE), OSHA, Toxic Hazard (TH) classifications, Hazardous Chemical Processes (including process calorimetry / thermal build up concepts). **3.2.3. Accreditations:** Accreditation of Laboratories, Introduction to ISO series, Indian Government Standards (ISI, Hallmark, Agmark) 3.2.4. **Good Laboratory Practices (GLP):** Principle, Objective, OECD guidelines, The US FDA 21CFR58, Klimisch score	
UNIT IV	**CALCULATIONS BASED ON CHEMICAL PRINCIPLES** **(The topics are to be covered in the form of numerical problems only.)**	**15L**

4.1	Concentration of a solution based on volume and mass units.	
4.2	Calculations of ppm, ppb and dilution of the solutions, concept of mmol.	
4.3	Stoichiometry of chemical reactions, concept of kg mol, limiting reactant, theoretical and practical yield.	
4.4	Solubility and solubility equilibria, effect of presence of common ions	
4.5	Calculations of pH of acids, bases, acidic and basic buffers.	
4.6	Concept of formation constants, stability and instability constants, stepwise formation constants.	
4.7	Oxidation number, rules for assigning oxidation number, redox reaction in term of oxidation number, oxidizing and reducing agents, equivalent weight of oxidizing and reducing agents, stoichiometry of redox titration (Normality of a solution of a oxidizing / reducing agent and its relationship with molarity).	

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3. Writing Reaction Mechanism in organic chemistry, A. Miller, P.H. Solomons, Academic Press.

4. Mechanism in Organic Chemistry, Peter sykes, 6th edition onwards.

5. Modern Methods of Organic Synthesis, W. Carruthers and Iain Coldham, Cambridge University Press.

6. Organic Synthesis, Jagdamba Singh, L.D.S. Yadav, PragatiPrakashan.

7. Stereochemistry: Conformation and mechanism, P.S. Kalsi, New Age International, New Delhi.

8.Stereochemistry of carbon compounds, E.L Eliel, S.H Wilen and L.N Manden, Wiley.

9. Stereochemistry of Organic Compounds- Principles and Applications, D. Nasipuri. New International Publishers Ltd

UNIT 3

1. Modern Analytical Chemistry by David Harvey, McGraw-Hill Higher Education

2. Principles of Instrumental Analysis - Skoog, Holler and Nieman, 5th Edition

3. Fundamentals of Analytical Chemistry, By Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, 9th Edition, 2004, Ch: 5.

4. Undergraduate Instrumental Analysis, 6th Edition, J W Robinson, Marcel Dekker, Ch:1.

5. ISO 9000 Quality Systems Handbook, Fourth Edition, David Hoyle. (Chapter: 3 & 4) (Free download).

6. Quality Control and Total Quality Management - P.L. Jain-Tata McGraw-Hill (2006) Total Quality Management - Bester field - Pearson Education, Ch:5.

7. OECD Principles of Good Laboratory Practice (as revised in 1997)". OECD Environmental Health and Safety Publications. OECD. 1. 1998.

UNIT 4

1. 3000 solved problems in chemistry, Schaum's Solved problem series, David E. Goldbers McGraw Hill international Editions, Chapter 11,15,16,21,22

NAME OF THE COURSE	**ORGANIC AND ANALYTICAL CHEMISTRY**	
CLASS	M.Sc Part 1	
COURSE CODE	SCHE512PMJ	
NUMBER OF CREDITS	2	
NUMBER OF LECTURES PER WEEK	4	
TOTAL NUMBER OF LECTURES PER SEMESTER	60	
EVALUATION METHOD	CONTINUOUS ASSESSMENT	SUMMATIVE EXAMINATION
TOTAL MARKS		50
PASSING MARKS	-----	20

PRACTICALS

Learning Objectives:Learner will learn

CO1	To synthesize organic compounds
CO2	To purify the given compound by suitable method
CO3	To learn analysis of individual and mixture of components by classical and instrumental methods learnt in theory
CO4	To learn the role of different solvents in sample pre-treatment to enhance accuracy of the

	result..
CO5	To get highly reproducible and accurate results irrespective of the origin of the sample.

Learning Outcomes:Learner will be able to

CLO1	Prepare organic compounds at micro scale
CLO2	To assess the purity of the prepared compound
CLO3	use concepts learnt in theory for solving practical problems.
CLO4	understand and apply the knowledge acquired in theory to different types of samples for its characterisation and estimation.
CLO5	be able to work comfortably at different concentrations with the highest degree of accuracy and reproducibility.

PRACTICALS

1. Anthracene to anthraquinone
2. Benzoin to benzil
3. Anthracene to Anthracene maleic anhydride adduct
4. 2-Naphthol to BINOL
5. p-Benzoquinone to 1,2,4-triacetoxybenzene
6. Ethyl acetoacetate to 3-methyl-1-phenylpyrazol-5-one
7. *o*-Phenylenediamine to 2-methylbenzimidazole

1. To determine (a) the ion exchange capacity (b) exchange efficiency of the given cation exchange resin.
2. To determine the amount of Cr(III) and Fe(II) individually in a mixture of the two by titration with EDTA.
3. To determine the breakthrough capacity of a cation exchange resin.
4. To determine the amount of Cu(II) present in the given solution containing a mixture of Cu(II) and Fe(II).

REFERENCES

1. Quantitative Inorganic Analysis including Elementary Instrumental Analysis by A. I. Vogel's, 3rd Ed.ELBS (1964)
2. Vogel's textbook of quantitative chemical analysis, Sixth Ed. Mendham, Denny, Barnes, Thomas,Pearson education
3. Standard methods of chemical analysis, F. J. Welcher
4. E.B.Sandell and H.Onishi,"Spectrophotometric Determination of Traces of Metals", Part II, 4th Ed., A Wiley Interscience Publication, New York,1978.

SOPHIA COLLEGE (AUTONOMOUS)

NAME OF THE COURSE	**Advanced Instrumental Techniques**	
CLASS	M.Sc Part 1	
COURSE CODE	SCHE511E	
NUMBER OF CREDITS	4	
NUMBER OF LECTURES PER WEEK	4	
TOTAL NUMBER OF LECTURES PER SEMESTER	60	
EVALUATION METHOD	CONTINUOUS ASSESSMENT	SUMMATIVE ASSESSMENT
TOTAL MARKS PASSING MARKS	50 20	50 20

Learning Objective

CO1	To learn about FTIR and UV-Vis spectroscopy as an analytical tool.
CO2	To understand application of different X-ray spectroscopic methods as a tool for surface studies
CO3	To learn the principle and working of MSwith different analysers as a tool for structural elucidation of organic compounds.

Learning Outcomes

CLO1	To be able to explain the working and applications of IR, FTIR and UV-Vis spectroscopy in various fields
CLO2	To be able to solve numerical problems on simultaneous spectroscopy.
CLO3	Explain various chromatographic X-ray spectroscopic methods with emphasis on applications of IR, FTIR and UV-Vis spectroscopy in various fields
CLO4	To be able to solve numerical problems on simultaneous spectroscopy.

UNIT I	**OPTICAL METHOD**	**15L**
1.1	**1.1**Recapitulation of basic concepts, Electromagnetic spectrum, Sources, Detectors, sample containers. **1.1.2** Laser as a source of radiation, Fibre optics **1.1.3** Introduction of Fourier transformer	
1.2	**1.2** Beer- Lambert's Law, factors affecting molecular absorption, types of transitions [emphasis on charge transfer absorption], pH, temperature, solvent and effect of substituents. Applications of Ultraviolet and Visible spectroscopy: **1.2.2** On charge transfer absorption Simultaneous spectroscopy	

	Derivative Spectroscopy Dual spectrometry – Introduction, Principle, Instrumentation and Applications	
1.3	**1.3.1** Instrumentation: Sources, Sample handling, Transducers, Dispersive, non-dispersive instrument **1.3.2** FTIR and its advantages **1.3.3** Applications of IR [Mid IR, Near IR, Far IR]: Qualitative with emphasis on "Finger print" region, Quantitative analysis, Advantages and Limitations of IR **1.3.4** Introduction and basic principles of diffuse reflectance spectroscopy.	
UNIT II	**SPECTROSCOPY AND RADIOANALYTICAL METHODS**	**15L**
2.1	Principle, instrumentation and applications of X-ray fluorescence, absorption and diffraction spectroscopy.	
2.2	Recapitulation, instrumentation, ion sources for molecular studies, electron impact, field ionization, field desorption, chemical ionization and fast atom bombardment sources. Mass analyzers: Quadrupole, time of flight and ion trap. Applications.	
2.3	Recapitulation, isotope dilution method, introduction, principle, single dilution method, double dilution method and application.	

REFERENCES

Unit 1

D. A. Skoog, F. J. Holler, T. A. Nieman, Principles of Instrumental Analysis, 5th Edition, Harcourt Asia Publisher. Chapter 6, 7.

H. H. Willard, L. L. Merritt, J. A. Dean, F. A. Settle, Instrumental Methods of Analysis,6 th Edition, CBS Publisher. Chapter 2.

R. D. Braun, Introduction to Instrumental Analysis, McGraw Hill Publisher. Chapter 8.

G. W. Ewing, Instrumental Methods of Chemical Analysis, 5 th Edition, McGraw Hill Publisher, Chapter 3.

M. Ito, The effect of temperature on ultraviolet absorption spectra and its relation to hydrogen bonding, J. Mol. Spectrosc. 4 (1960) 106-124

Unit 2

Essentials of Nuclear Chemistry, H J Arnikar, New Age Publishers (2005)

Fundamentals of Radiochemistry D. D. Sood , A. V. R. Reddy and N. Ramamoorthy

Principles of Instrumental Analysis - Skoog, Holler and Nieman, 5th Edition, Ch: 12

PRACTICALS

Learning Objectives

CO1	To learn handling of different instruments.
CO2	To use a given method to comment on the quality of the compound.

Learning Outcomes: The learner will be able to

CLO1	Check the quality of any given compound.
CLO2	handle various instruments confidently.
CLO3	perform analysis at various concentrations.

PRACTICAL

1.To determine percentage composition of saline injection. Estimation of sodium chloride by Volhard's method and glucose by polarimetry.

2.To estimate Vitamin B_{12} /fluorescein by fluorimetry.

3.Simultaneous determination of Cr(VI) and Mn(VII) in a mixture spectrophotometrically

4.To determine the percentage purity of a sample (glycine/sodium benzoate/primary amine/ajino motto) by titration with perchloric acid in a non- aqueous medium using a glass calomel system potentiometrically.

5.To determine the amount of Fe(II) and Fe(III) in a mixture using 1,10-phenanthroline

spectrophotometrically.

6.To determine the amount of calcium in milk powder by flame photometry.

7.Determination of K^+ in a given sample by standard addition method (flame photometer)

8. Spectral interpretation of IR, mass and XRD spectrum

REFERENCES

1. Quantitative Inorganic Analysis including Elementary Instrumental Analysis by A. I. Vogels, 3rd Ed. ELBS (1964)
2. Standard Instrumental Methods of Chemical Analysis, F. J. Welcher

NAME OF THE COURSE	Research Methodology	
CLASS	M.Sc Part 1	
COURSE CODE	SCHE11RM	
NUMBER OF CREDITS	4	
NUMBER OF LECTURES PER WEEK	4	
TOTAL NUMBER OF LECTURES PER SEMESTER	60	
EVALUATION METHOD	CONTINUOUS ASSESSMENT	SUMMATIVE ASSESSMENT
TOTAL MARKS PASSING MARKS	50 20	----

Learning objectives

CO1	
CO2	
CO3	

Learning Outcomes:

CLO1	
CLO2	
CLO3	

UNIT I	**SCIENTIFIC INVESTIGATION**	**15L**

1.1	Measurement and errors: Introduction to measurement; errors and types of errors (gross, systematic and random) with examples and case studies; uncertainty in measurement- accuracy, precision (definition and their estimation), significant figures.	
1.2	Describing Data: Analytical Data, population and sample; measures of central tendencies-mean, median; measures of dispersion or variability- standard deviation, variance, RSD; degrees of freedom and standard deviation of mean; confidence intervals and confidence limits; repeatability and reproducibility of measurement.	
1.3	ICH guidelines for analytical procedures- Introduction to analytical procedure development; Validation of analytical procedures: Specificity, linearity, range, accuracy, precision, detection and quantitation limits, robustness and system suitability testing	
1.4	Scientific Literature and communication: Print, digital, information technology and library resources; scientific reporting of practical and project work, literature review, oral and poster presentations, manuscript- title, abstract and body IMRaD format, acknowledgements and references; scientific misconduct- falsification, fabrication and plagiarism, authorship and ethics in scientific research	
UNIT II	**DATA REPRESENTATION AND INTERPRETATION**	**15L**
2.1	Representation of data: Figures and Tables; Graphs, pictographs, scatter plots; file formats resolution and legends.	
2.2	Testing of hypotheses: Importance of hypotheses testing, levels of confidence and significance, type I & II errors, determining significant systematic errors- Z, t test; normal distribution; testing of means- student's t test; testing Variances- F test, ANOVA.	
2.3	Advanced statistical techniques & calibration: Correlation and regression, curve fitting, linear calibration model, analysis of residuals, interpolation through linear least square fitting, r and r squared.	
2.4	Polynomial fitting and Multivariate analysis: general polynomial fitting, linearizing transformations, exponential function fit, basic aspects of multiple linear regression analysis, discriminant analysis, multivariate analysis of variance, factor and cluster analysis.	
UNIT III	**LABORATORY SAFETY & ETHICAL HANDLING OF CHEMICALS**	**15L**
3.1	Principles, ethics and safety practices: Hazards, risk and safety; RAMP principles of safety; safety ethics and rules	
3.2	Sustainable and green practices in the laboratory: green chemistry principles and practices	
3.3	Safety regulations: employers expectations of safety skills; laws and regulations pertaining to safety- 29CFR, Indian CMSR (Chemical Management and Safety Rules)	

3.4	Understanding laboratory hazards: Signs, symbols and safety; Hazard information (MSDS, SDS); Globally Harmonized System of Classification and Labelling of Chemicals (GHS); physical hazards in the laboratory and their minimization (case studies)	
UNIT IV	**LOGICAL MATHEMATICAL REASONING & COMPUTATIONAL TOOLS**	**15L**
4.1	Types of reasoning; Number series, Letter series, Codes and Relationships; Mathematical Aptitude (Fraction, Time & Distance, Ratio, Proportion and Percentage, Profit and Loss, Interest and Discounting, Averages etc.)	
4.2	Microsoft excel and origin for Chemists: Determination of central tendencies and dispersion- mean, standard deviation, RSD; confidence limits; plots using excel & origin, correlation and regression, standard errors, error bars	
4.3	Use of excel in analytical chemistry: titration curves and determination of equivalence points, derivative plots; simulation of chemical kinetics	
4.4	Cheminformatics tools: Chemdraw, Chemsketch, Mestrenova, NMRDB, openbabel,Reference manager (Mendeley)	

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Unit 1
1. Hibbert, D. B. & Gooding, J. J. (2006) Data Analysis for Chemistry Oxford University Press
2. Dharmapalan, B. (2012). Scientific Research Methodology. Alpha Science International Ltd.
3. International Council of Harmonisation: https://www.ich.org/page/quality-guidelines

Unit 2
1. Hibbert, D. B. & Gooding, J. J. (2006) Data Analysis for Chemistry Oxford University Press
2. Chandra S. & Sharma M. K. (2013). Research methodology. Alpha Science International.
3. Kothari C. R. (2004). Research methodology : methods & techniques (2nd rev.). New Age International (P).

Unit 3.
1. Hill R. H. & Finster D. C. (2016). Laboratory safety for chemistry students (Second). John Wiley & Sons.
2. Indian Chemical Regulation https://indianchemicalregulation.com/
3. American Chemical Society https://institute.acs.org/courses.html

Unit 4
1. K.V.S. Madaan (2020). Teaching and Research Aptitude, Pearson India Education Services Pvt. Ltd

2. Levie, R. D. (2012, June 5). How to Use Excel® in Analytical Chemistry: And in General Scientific Data Analysis, Cambridge University Press
3. Skoog, D. A., West, D. M., Holler, F. J., & Crouch, S. R. (2021, May 14). Applications of Microsoft Excel in Analytical Chemistry.
4. Levie, R. D. (2012, June 5). How to Use Excel® in Analytical Chemistry: And in General Scientific Data Analysis. Brooks/Cole Cengage Learning
5. Hibbert, D. B. & Gooding, J. J. (2006) Data Analysis for Chemistry Oxford University press

SEMESTER -II

NAME OF THE COURSE	PHYSICAL AND INORGANIC CHEMISTRY	
CLASS	M.Sc PART 1	
COURSE CODE	SCHE523PMJ	
NUMBER OF CREDITS	4	
NUMBER OF LECTURES PER WEEK	4	
TOTAL NUMBER OF LECTURES PER SEMESTER	60	
EVALUATION METHOD	CONTINUOUS ASSESSMENT	SUMMATIVE ASSESSMENT
TOTAL MARKS PASSING MARKS	50 20	50 20

Course Objectives

CO1	To understand and elucidate the properties of wave function, quantum operators and application of quantum mechanics to different systems.
CO2	To study Debye Huckel Onsager equation, deviations from it and to understand different types of fuel cells.
CO3	To understand different types of reactions and their mechanisms for inorganic complexes of varying geometry
CO4	To explore the structure, bonding and reactivity of organometallic compounds involving transition metals

Course Outcomes:The learner will be able to

CLO1	Explain and use Quantum operators in solving numericals
CLO2	Elucidate Debye Huckel Onsager equation, Debye Falkenhagen effect, Wein effect
CLO3	Identify different types of reactions and their mechanisms for inorganic complexes of varying geometry
CLO4	Comprehend the unique bonding and structural features of organometallic compounds of transition metals and predict the reactivity

SOPHIA COLLEGE (AUTONOMOUS)

UNIT I	**QUANTUM CHEMISTRY**	**15L**
1.1	Classical Mechanics, failure of classical mechanics, Need for Quantum mechanics.	
1.2	Particle waves and Schrödinger wave equation, wave functions, properties of wave functions, Normalization of wave functions,orthogonality of wave functions.	
1.3	Operators and their algebra, linear and Hermitian operators, operators for the dynamic variables of a system such as, position, linear momentum, angular momentum, total energy, Eigen functions, Eigen values and Eigen value equation, Schrödinger wave equation as the Eigen value equation of the Hamiltonian operator, average value and the expectation value of a dynamic variable of the system, Postulates of Quantum Mechanics, Schrodinger's Time independent wave equation from Schrodinger's time dependent wave equation.	
1.4	Application of quantum mechanics to the following systems: a) Free particle, wave function and energy of a free particle. b) Particle in a one, two and three dimensional box, separation of variables, Expression for the wave function of the system, expression for the energy of the system, concept of quantization, introduction of quantum number, degeneracy of the energy levels. c) Harmonic oscillator, approximate solution of the equation, Hermite polynomials, expression for wave function, expression for energy,use of the recursion formula.	
UNIT II	**ELECTROCHEMISTRY**	**15L**
2.1	Debye-Hückel theory of activity coefficient, Debye-Hückel limiting law and it's extension to higher concentration (derivations are expected)	
2.2	Electrolytic conductance and ionic interaction, relaxation effect. Debye-Hückel-Onsager equation (derivation expected). Validity of this equation for aqueous and non- aqueous solution, deviations from Onsager equation, Debye-Falkenhagen effect (dispersion of conductance at high frequencies), Wien effect.	
2.3	Batteries: Types of fuel cells- Alkaline fuel cells, Phosphoric acid fuel cells, High temperature fuel cells [Solid –Oxide Fuel Cells (SOFC) and Molten Carbonate Fuel Cells]- Principle, construction and working, application in transportation.	
UNIT III	**INORGANIC REACTION MECHANISM**	**15L**
3.1	Rate of reactions, factors affecting the rate of reactions, techniques for determination of rate of reaction (Direct chemical analysis, spectrophotometric method, electrochemical and flow methods).	
3.2	Ligand substitution reactions of: (Mechanism and factors affecting these	

	substitution reactions.) a) Octahedral complexes without breaking of metal-ligand bond (Use of isotopic labelling method) b) Square planar complexes, trans-effect, its theories and applications. c) Tetrahedral complexes.	
3.3	Redox reactions: electron and atom transfer, inner and outer sphere mechanisms, complementary and non-complimentary reactions.	
3.4	Stereochemistry of substitution reactions of octahedral complexes. (Isomerization and racemization reactions and applications.)	
UNIT IV	**ORGANOMETALLIC CHEMISTRY OF TRANSITION METALS**	**15L**
4.1	Eighteen and sixteen electron rule - comparison and electron counting with examples.	
4.2	Preparation, reactions and properties of the following compounds (a) Alkyl and aryl derivatives of Pd and Pt complexes (b) Carbenes and carbynes of Cr, Mo and W (c) Alkene derivatives of Pd and Pt (d) Alkyne derivatives of Pd and Pt (e) Allyl derivatives of nickel (f) Sandwich compounds of Cr and Half Sandwich compounds of Cr, Mo.	
4.3	Structure and bonding on the basis of VBT and MOT in the following organometallic compounds: Zeise's salt, bis(triphenylphosphine)diphenylacetylene platinum(0) $[Pt(PPh_3)_2(HC{\equiv}CPh)_2]$, diallyl nickel(II), ferrocene and bis(arene)chromium(0), tricarbonyl (η_2-butadiene) iron(0).	

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Ira R. Levine, Physical Chemistry, 5th Edition, Tata McGraw-Hill New Delhi, 2002.

G.W. Castellan, Physical Chemistry, 3rd Edition, Narosa Publishing House, New Delhi, 1983.

S. Glasstone, Textbook of Physical Chemistry, 2ndEdition., McMillan and Co. Ltd., London, 1962

Thomas Engel and Philip Reid, Physical Chemistry, 3rd Edition, Pearson Education Limited 2013.

D.N. Bajpai, Advanced Physical Chemistry, S. Chand 1st Edition, 1992.

Bockris, John O'M., Reddy, Amulya K.N., Gamboa-Aldeco, Maria E., Modern Electrochemistry, 2A, Plenum Publishers, 1998.

Physical Chemistry by Gurtu and Gurtu

A Textbook of Physical Chemistry by K L kapoorVol 5, 2ndEdition

P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Inorganic Chemistry, 5 th Ed., Oxford University Press, 2010.

10. W. H. Malik, G. D. Tuli and R. D. Madan, Selected Topics in Inorganic Chemistry, 8th Ed., S. Chand & Company ltd.

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12. S. Asperger, Chemical kinetics and Inorganic Reaction Mechanism, 2nd Ed., Kluwer Academic/Plenum Publishers, 2002

13. F. Basalo and R. G. Pearson, Mechanism of Inorganic Reactions, 2nd Ed., Wiley, 1967.

14. R. Gopalan and V. Ramlingam, Concise Coordination chemistry, Vikas Publishing house Pvt Ltd., 2001.

15. Robert B. Jordan, Reaction Mechanisms of Inorganic and Organometallic Systems, 3rd Ed.,Oxford University Press 2008

16. D. Banerjea, Coordination chemistry. Tata McGrew Hill, New Delhi,1993.

17. R.C Mehrotra and A.Singh, Organometallic Chemistry- A unified Approach, 2nded, New Age International Pvt Ltd, 2000.

18. R.H Crabtree, The Organometallic Chemistry of the Transition Metals, 5th edition, Wiley International Pvt, Ltd 2000.

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20. Organometallic Chemistry by G.S Sodhi. Ane Books Pvt Ltd.

PRACTICALS

NAME OF THE COU	PHYSICAL AND INORGANIC CHEMISTRY

SOPHIA COLLEGE (AUTONOMOUS)

RSE	
CLASS	M.Sc PART 1
COURSE CODE	SCHE523PMJ
NUMBER OF CREDITS	2
NUMBER OF LEC	4

TURES PER WEEK	
TOTAL NUMBER OF LECTURES PER SEMEST	60

SOPHIA COLLEGE (AUTONOMOUS)

ER		
EVALUATION METHOD TOTAL MARKS PASSING MARKS	CONTINUOUS ASSESSMENT -----	SUMMATIVE ASSESSMENT 5020

COURSE OBJECTIVE

CO1	To train the students in handling various instruments, glassware, chemicals etc. used in various analyses
CO2	To instruct the learner in practical knowledge on planning and performing experiments.
CO3	To elucidate knowledge about the non-instrumental techniques.
CO4	To understand the methods of preparation and properties of co-ordination compounds
CO5	To understand different types of reactions and their mechanisms for inorganic complexes of varying geometry.

COURSE OUTCOMES: The learner will be able to:

CLO1	carefully handle and use various instruments used in the laboratory for performing experiments
CLO2	follow instructions thoroughly
CLO3	perform experiments with accuracy and perfection
CLO4	identify different types of reactions and their mechanisms for inorganic complexes of varying geometry.
CLO5	write the methods of preparation and explain the properties of coordination compounds.

Non-Instrumental

1.Study the variation in the solubility of $Ca(OH)_2$ in presence of NaOH and to determine the solubility product of $Ca(OH)_2$ at room temperature.

2. To investigate the reaction between acetone and iodine.

3. Polar plots of atomic orbitals such as s, p and dz^2orbitals by using angular plots of hydrogen atom wave functions.

Instrumental

1. Study the effect of substituent on the dissociation constant of acetic acid conductometrically.

2. Determine the formula of silver ammonia complex by potentiometric method.

I] Inorganic Preparations (Synthesis and Characterization)

1) Bis-(tetraethylammonium) tetrachlorocuprate (II)- $(Et_4\ N)_2[CuCl_4]$

2) Bis-(tetraethylammonium)tetrachloronickelate(II)- $(Et_4\ N)_2\ [NiCl_4]$

3) Tetramminemonocarbanato cobalt (III) nitrate- $[Co(NH_3)_4CO_3]NO_3$

4) Hydronium dichlorobis(dimethylglyoximato) cobaltate(III)- $H[Co(dmgH)_2Cl_2\ ]$

5) Bis (ethylenediammine) copper (II) sulphate- $[Cu(en)_2]SO_4$

II] Instrumentation

1) Determination of equilibrium constant by Slope intercept method for Fe^{+3} / SCNsystem.

REFERENCE

1.Advanced experiments in Inorganic Chemistry., G. N. Mukherjee., 1stEdition., 2010., U.N.Dhur& Sons Pvt Ltd

2.The Synthesis and Characterization of Inorganic Compounds by William L. Jolly

3.Inorganic Chemistry Practical Under UGC Syllabus for M.Sc. in all India Universities By:Dr Deepak Pant

4.Practical Physical Chemistry, B. Viswanathan and P.S. Raghavan, Viva Books Private Limited, 2005.

5.Practical Physical Chemistry, A.M. James and F.E. Prichard, 3rd Edition, Longman Group Ltd., 1974.

6.Experimental Physical Chemistry, V.D. Athawale and P. Mathur, New Age International Publishers, 2001

NAME OF THE COURSE	**ORGANIC AND ANALYTICAL CHEMISTRY**	
CLASS	M.Sc Part 1	
COURSE CODE	**SCHE524MJ**	
NUMBER OF CREDITS	4	
NUMBER OF LECTURES PER WEEK	4	
TOTAL NUMBER OF LECTURES PER SEMESTER	60	
EVALUATION METHOD	CONTINUOUS ASSESSMENT	SUMMATIVE ASSESSMENT
TOTAL MARKS PASSING MARKS	50 20	50 20

Course Objectives

CO1	Understanding chemical reactions with the help of FMO.
CO2	Understanding HOMO - LUMO gap in UV absorption spectra and interpreting there activity of

	the given compounds.
CO3	Learn the mechanisms and selectivity of the various rearrangement reactions
CO4	Know the basic concepts of Molecular spectroscopy.
CO5	To learn about DSC, DTA and thermometric titration methods as a method for the characterisation of various substances
CO6	To learn about advanced electroanalytical methods to analyse mixtures.

Course Outcomes:Learner will be able to:

CLO1	draw the FMO's of alkenes, Formaldehyde, allyl anion and cation.
CLO2	apply the concept of FMO's to substitution and addition reactions.
CLO3	predict whether the reaction is chemically/ photochemically feasible
CLO4	analyse the effect of certain factors on the spectrum of the compound
CLO5	interpretation of spectral data and elucidation of structure.
CLO6	explain various types of electroanalytical methods and compare advantages and limitations of one over the other.
CLO7	interpret thermograms of various compounds for identification and quantification.

UNIT I	**REACTIONS AND REARRANGEMENTS**	**5L**
	Mechanisms, stereochemistry (if applicable) and applications of the following: 1.1.1 Reactions: Baylis-Hilman reaction,Corey-Fuchs reaction, Nef reaction, Passerini reaction. 1.1.2 Concerted rearrangements: Wolff, Boulton Katritzky. 1.1.3 Cationic rearrangements:Tiffeneau-Demjanov, Pummerer, Dienone-phenol, Rupe. 1.1.4 Anionic rearrangements: Von Richter, Gabriel–Colman	
1.2	**MOLECULAR ORBITAL THEORY**	**10L**
	1.2.1 Molecular orbitals: Formation of σ- and π-MOs by using LCAO method. Formation of π MOs of ethylene, butadiene, 1, 3, 5-hexatriene,. Concept of nodal planes and energies of π-MOs 1.2.2 The Salem-Klopman equation. (no derivation expected) Explanation of the three terms in the equation. Hard and Soft Electrophiles and Nucleophiles. Examples of hard and soft nucleophiles/ electrophiles. Identification of hard and soft	

	reactive sites on the basis of MOs. 1.2.3 Introduction to FMOs: HOMO and LUMO and significance of HOMO-LUMO gap in absorption spectra. HOMO and LUMO in MO of allyl cation, anion and radical and regioselectivity in the chemical reactions of allyl cation with allyl anion. 1.2.4 MOs of formaldehyde: The effect of electronegativity perturbation and orbital polarization in formaldehyde. HOMO and LUMO (π and π^* orbitals) of formaldehyde. Perturbation Theory of Reactivity. Addition of hydride to formaldehyde. Orbital Symmetry, considerations for photochemical reactions of Alkenes and Dienes, photochemical electrocyclic reactions	
UNIT II	**SPECTROSCOPY**	**15L**
2.1	Ultraviolet spectroscopy: Recapitulation - UV spectra of dienes, conjugated polyenes (cyclic and acyclic), carbonyl and unsaturated carbonyl compounds, substituted aromatic compounds. Factors affecting the position and intensity of UV bands – effect of conjugation, steric factor, pH, and solvent polarity. Calculation of absorption maxima for above classes of compounds by Woodward-Fieser rules (using Woodward-Fieser tables for values for substituents).	
2.2	Infrared spectroscopy: Fundamental, overtone and combination bands, vibrational coupling, factors affecting vibrational frequency (atomic weight, conjugation, ring size, solvent and hydrogen bonding). Characteristic vibrational frequencies for alkanes, alkenes, alkynes, aromatics, alcohols, ethers, phenols, amines, nitriles and nitro compounds. Detailed study of vibrational frequencies of carbonyl compounds, aldehydes, ketones, esters, amides, acids, acid halides, anhydrides, lactones, lactams and conjugated carbonyl compounds.	
2.3	Proton magnetic resonance spectroscopy: Principle, Chemical shift, Factors affecting chemical shift (Electronegativity, H-bonding, Anisotropy effects). Chemical and magnetic equivalence, Chemical shift values and correlation for protons bonded to carbon and other nuclei as in alcohols, phenols, enols, carboxylic acids, amines, amides. Spin-spin coupling, Coupling constant (J), Factors affecting J, geminal, vicinal and long range coupling (allylic and aromatic). First order spectra, Karplus equation. ^{13}C NMR spectroscopy: Theory and comparison with proton NMR, proton coupled and decoupled spectra, off-resonance decoupling. Factors influencing carbon shifts, correlation of chemical shifts of aliphatic, olefin, alkyne, aromatic and carbonyl carbons.	
2.4	Mass spectrometry: Molecular ion peak, base peak, isotopic abundance, Nitrogen rule, Rule of 13. Determination of molecular formula of organic compounds based on isotopic	

	abundance and HRMS. Fragmentation pattern in various classes of organic compounds (including compounds containing hetero atoms), McLafferty rearrangement, Retro-Diels-Alder reaction. Structure determination involving individual or combined use of the above spectral techniques.	
UNIT III	**THERMAL METHODS**	**15L**
3.1	3.1.1.Introduction: Recapitulation of types of thermal methods, comparison between TGA and DTA. 3.1.2 Differential Scanning Calorimetry: Principle, comparison of DTA and DSC, Instrumentation, Block diagram, Nature of DSC Curve, Factors affecting curves (sample size, sample shape, pressure). 3.1.3 Applications: Heat of reaction, Specific heat, Safety screening, Polymers, liquid crystals, Percentage crystallinity, oxidative stability, Drug analysis, Analysis of Polyethylene for its crystallinity.	
3.2	Thermometric titrations: Introduction, instrumentation, applications in the titration of (i) HCl Vs NaOH (ii) Boric acid Vs NaOH (iii) A mixture of Ca^{2+} and Mg^{2+}Vs EDTA (iv) Zn^{2+} with disodium tartarate.	
UNIT IV	**ELECTROANALYTICAL METHODS**	**15L**
4.1	Ion selective potentiometry and Polarography: 4.1.1.Ion selective potentiometry: Ion selective electrodes and their applications (solid state, precipitate, liquid –liquid, enzyme and gas sensing electrodes), ion selective field effect transistors, biocatalytic membrane electrodes and enzyme based biosensors. 4.1.2 Polarography: Ilkovic equation, derivation starting with Cottrell equation, effect of complex formation on the polarographic waves.	
4.2	Electrogravimetry: Introduction, principle, instrumentation, factors affecting the nature of the deposit and applications.	
4.3	Coulometry: Introduction, principle, instrumentation, coulometry at controlled potential and controlled current.	
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SOPHIA COLLEGE (AUTONOMOUS)

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2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Part A, page no. 713-769, and B, Plenum Press.

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4. Organic Chemistry, R.T. Morrison, R.N. Boyd and S.K. Bhattacharjee, Pearson Publication (7th Edition)

5. Advanced Organic Chemistry: Reactions and mechanism, B. Miller and R. Prasad, Pearson Education.

6. Advanced Organic Chemistry: Reaction mechanisms, R. Bruckner, Academic Press.

7. Understanding Organic Reaction Mechanisms, Adams Jacobs, Cambridge University Press.

8. Writing Reaction Mechanism in organic chemistry, A. Miller, P.H. Solomons, Academic Press.

9. Principles of Organic Synthesis, R.O.C. Norman and J.M Coxon, Nelson Thornes.

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14. Spectrometric Identification of Organic Compounds, R. Silverstein, G.C Bassler and T.C. Morrill, JJohn Wiley and Sons.

15. Introduction to instrumental methods of analysis by Robert D. Braun, Mc. Graw Hill (1987): Chapter 27

16. Thermal Analysis-theory and applications by R. T. Sane, Ghadge, Quest Publications

17. Instrumental methods of analysis, 7 th Edition, Willard, Merrit, Dean: Chapter 25

18. Instrumental Analysis, 5 th Edition, Skoog, Holler and Nieman: Chapter 31

19. Quantitative Chemical Analysis, 6 th Edition, Vogel: Chapter 12

20. Analytical Chemistry by Open Learning: Thermal Methods by James W. Dodd & Kenneth H. Tonge

21. Principles of Instrumental Analysis – Skoog, Holler, Nieman, 5th Edition, Harcourt College Publishers, 1998. Chapters - 23, 24, 25.

22. Modern Analytical Chemistry David Harvey; McGraw Hill Higher education publishers, (2000).

23. Vogel's Textbook of quantitative chemical analysis, 6th edition, Pearson Education Limited, (2007).

24. Electrochemical Methods Fundamentals and Applications, Allen J Bard and Larry R Faulkner, John Wiley and Sons, (1980).

25. Instrumental Methods of Analysis Willard, Merrit, Dean and Settle, 7th edition, CBS publishers

PRACTICALS

NAME OF THE COURSE	ORGANIC AND ANALYTICAL CHEMISTRY	
CLASS	M.Sc Part 1	
COURSE CODE	SCHE524PMJ	
NUMBER OF CREDITS	2	
NUMBER OF LECTURES PER WEEK	4	
TOTAL NUMBER OF LECTURES PER SEMESTER	60	
EVALUATION METHOD	CONTINUOUS ASSESSMENT	SUMMATIVE ASSESSMENT
TOTAL MARKS PASSING MARKS	----	50 20

COURSE OBJECTIVE:Learner will

CO1	Learn to perform qualitative analysis, prepare a derivative and identify one of the components
CO2	Learn the method of purification of components.
CO3	To learn analysis of individual and mixture of components by classical and instrumental methods learnt in theory.
CO4	To learn the role of different solvents in sample pre-treatment to enhance accuracy of the result..
CO5	To get highly reproducible and accurate results irrespective of the origin of the sample.

COURSE OUTCOMES:Learner will be able:

CLO1	To identify the nature of a binary mixture and separate the mixture quantitatively.
CLO2	To perform organic qualitative analysis

CLO3	To purify compounds by distilling/recrystallization techniques
CLO4	use concepts learnt in theory for solving practical problems.
CLO5	understand and apply the knowledge acquired in theory to different types of samples for its characterisation and estimation.
CLO6	be able to analyse samples of different concentrations with the highest degree of accuracy and reproducibility.

Separation of Binary mixture using micro-scale technique

1. Separation of binary mixture using physical and chemical methods.
2. Characterization of one of the components with the help of chemical analysis and confirmation of the structure with the help of derivative preparation and its physical constant.
3. Purification and determination of mass and physical constant of the second component. The following types are expected:
a) Water soluble/water insoluble solid and water insoluble solid,
b) Non-volatile liquid-Non-volatile liquid (chemical separation)
c) Water-insoluble solid-Non-volatile liquid.

1.To determine the percentage composition of HCl and H2SO4 on weight basis in a mixture of two by conductometric titration with NaOH and BaCl2.
2.To determine the amount of nitrite in the given water sample.
3.To determine the amount of Fe(III) in the given solution by photometric titration using EDTA.
4.Determination of Ni spectrophotometry using dimethylglyoxime.

REFERENCES

1. Quantitative Inorganic Analysis including Elementary Instrumental Analysis by A. I. Vogels, 3 rd Ed. ELBS (1964)
2. Standard Instrumental Methods of Chemical Analysis, F. J. Welcher.
3.Systematic Qualitative organic analysis, H. Middleton (Orient Longman)
4. A Handbook of Organic Analysis, H.T. Clark (Orient Longman)
5. Systematic Identification of organic compounds, R.L. Shriner (John Wiley, New York)
6. Practical Organic Chemistry by Mann and Saunders.
7. Advance Practical Organic Chemistry, N.K. Vishnoi, Vikas Publication

NAME OF THE COURSE	Advanced Instrumental Techniques
CLASS	M.Sc Part 1
COURSE CODE	SCHE522E
NUMBER OF CREDITS	2

SOPHIA COLLEGE (AUTONOMOUS)

NUMBER OF LECTURES PER WEEK	4	
TOTAL NUMBER OF LECTURES PER SEMESTER	60	
EVALUATION METHOD	CONTINUOUS ASSESSMENT	SUMMATIVE ASSESSMENT
TOTAL MARKS	50	-
PASSING MARKS	20	-

Course Objectives

CO1	To understand application of different X-ray spectroscopic methods as a tool for surface studies.
CO2	To learn the principle and working of various chromatographic methods for separation and identification of mixture of unknown compounds by using suitable detectors.

Course Outcomes:The learner will be able to:

CLO1	explain various chromatographic, ICP-AES and X-ray spectroscopic methods with emphasis on principle and working of the instrument.
CLO2	draw a simple block/schematic diagram of the instruments learnt and explain the importance of each component.

UNIT I	**SURFACE ANALYTICAL TECHNIQUE**	
1.1	Surface Analytical Techniques: Introduction, Principle, Instrumentation and Applications of: 1.1.1 Scanning Electron Microscopy (SEM) 1.1.2 Scanning Tunnelling Microscopy (STM) 1.1.3 Transmission Electron Microscopy (TEM) 1.1.4 Electron Spectroscopy (ESCA and Auger)	**15L**
1.2	Atomic Spectroscopy:Introduction, Principle, Instrumentation and Applications. 1.2.1 Advantages and Limitations of AAS 1.2.2 Atomic Spectroscopy based on plasma sources	
Chromatography		**15L**
2.1	Concept of plate and rate theories in chromatography: efficiency, resolution, selectivity and separation capability. Van Deemter equation and broadening of chromatographic peaks. Optimization of chromatographic conditions.	
2.2	Gas Chromatography: Instrumentation of GC with special reference to sample injection systems – split/splitless, column types, solid/ liquid stationary phases, column switching techniques, temperature programming, Thermionic and mass spectrometric detector, Applications.	

2.3	HPTLC: Introduction to HPTLC, techniques in HPTLC. Determination by detectors: single beam densitometer, double beam densitometer, fluorimetric detector. Comparison between TLC and HPTLC. Advantages, limitations and applications of HPTLC	
2.4	Size exclusion chromatography: Basic principle and applications in the field of polymers	

REFERENCE

1. Physical Principles of Electron Microscopy, An Introduction to TEM, SEM, and AEM

2. Authors: Ray F. Egerton, ISBN: 978-0- 387-25800- 3 (Print) 978-0- 387-26016- 7 (Online)

3. Modern techniques of surface science by D.P. Woodruff, T.A. Delchar, Cambridge Univ. Press, 1994.

4. Introduction to Scanning Tunneling Microscopy by C. J. Chen, Oxford University Press, NewYork, 1993.

5. Transmission Electron Microscopy: A text book for Material Science, David B Williams and C., Barry Carter, Springer

6. Modern Spectroscopy, by J.M. Hollas, 3rd Edition (1996), John Wiley, New York

7. Principles of Instrumental Analysis – Skoog, Holler, Nieman, 5th ed., Harcourt College Publishers, 1998.

8.Instrumental Analysis, Skoog, Holler & Crouch

9. HPTLC Analysis: Dilip Charegaonkar

PRACTICALS

SOPHIA COLLEGE (AUTONOMOUS)

COURSE OBJECTIVES

CO1	To learn working and applications of different instruments.
CO2	To use a given method to comment on the quality of the compound.

COURSE OUTCOMES:The learner will be able to:

CLO1	Check the quality of any given compound.
CLO2	handle various instruments confidently.
CLO3	perform analysis at various concentrations.

1.To determine the amount of nitro group by the titanium method.

2. Estimation of Vitamin C by titration with potassium borate.

3. Determination of pKa value of phosphoric acid by photometric titration with sodium hydroxide using glass electrode.

4. Separation and estimation of Zn (II) and Ni (II) in a mixture, using an anion exchanger.

5.Estimation of a mixture of hydrochloric acid and boric acid by acid base titration.

REFERENCE

Quantitative Inorganic Analysis including Elementary Instrumental Analysis by A. I. Vogels, 3rd Ed. ELBS (1964)

Standard Instrumental Methods of Chemical Analysis, F. J. Welcher

Assessment pattern

For Major papers

I.CONTINUOUS ASSESSMENT IA: 50 MARKS

1-ACTIVITY 25 MARKS

1-TEST 25 MARKS

II. SUMMATIVE ASSESSMENT (SEE): 50 MARKS (SUBJECTIVE)

All units of the syllabus will be covered in SEE and will be given equal weightage.

Q.1. Unit 1 (A): Attempt any two of the following. (2 out of 4) [10marks]

Q.2. Unit 2 (A): Attempt any two of the following. (2 out of 4) [10marks]

Q.3. Unit 3 (A): Attempt any two of the following. (2 out of 4) [10marks]

Q.4. Unit 4 (A): Attempt any two of the following. (2 out of 4) [10marks]

Q.5. Attempt any two of the following (2 out of 4) [10 marks]

(1 question from each unit)

SOPHIA COLLEGE (AUTONOMOUS)

III.CONTINUOUS ASSESSMENT(For Elective paper)
DSE
1.CONTINUOUS ASSESSMENT IA: 50 MARKS
2 Subjective test of 25 marks each
RM
1. CONTINUOUS ASSESSMENT IA : 50 MARKS
2. 1 Subjective test of 25 marks
3. Assignment activity of 25 marks

IV. PRACTICAL EXAMINATION
A 50 marks practical examination will be conducted at the end of the semester for 50 marks.

CA, SA and Practical are separate heads of passing. The learner will have to get 20 out of 50 to pass the examination.

Practical 40M
Journal 5M
Viva-voce 5M
Total 50M