Programme Outline: MSc (SEMESTER I)



MUMBAI

Programme: Science

Programme Code:

SMSCHE

M.Sc. Part

I

(Choice Based Credit System with effect from the year 2018-19)

Programme Outline: MSc (SEMESTER II)

Course Code	Unit No	Name of the Unit	Credits
SMSCHE201		PHYSICAL CHEMISTRY	4
	1	Thermodynamics – II	
	2	Quantum Chemistry – II	
	3	Chemical Dynamics – II	
	4	Solid State Chemistry and Phase	
		Equilibria	
SMSCHE202		INORGANIC CHEMISTRY	4
	1	Inorganic Reaction Mechanism	
	2	Organometallic Chemistry of Transition metals	
	3	Environmental Chemistry	
	4	Bioinorganic Chemistry	
SMSCHE203		ORGANIC CHEMISTRY	4
	1	Alkylation and reaction of carbon	
		nucleophiles	
	2	Reactions and Rearrangements	
	3	Molecular Orbital Theory and UV-IR	
		Spectrometery	
	4	NMR and Mass Spectrometry	
SMSCHE204		ANALYTICAL CHEMISTRY	4
	1	Chromatography	
	2	Spectrometry and Radio-Analytical	
		methods	
	3	Surface Analytical techniques	
	4	Electroanalytical methods	
SMSCHEP201		PHYSICAL CHEMISTRY	2
		PRACTICAL	
SMSCHEP202		INORGANIC CHEMISTRY 2	
		PRACTICAL	
SMSCHEP203		ORGANIC CHEMISTRY PRACTICAL	2
SMSCHEP204		ANALYTICAL CHEMISTRY	2
		PRACTICAL	

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 the theoretical and applied knowledge in the inter disciplinary		
	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 issue and face the real life		
	challenges more effectively.		

PROGRAMME SPECIFIC OUTCOMES

PSO 1	Critical thinking: A student with 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.

SEMESTER 1

NAME OF THE COURSE	PHYSICAL CHEMIST	RY
CLASS	MSC	
COURSE CODE	SMSCHE101	
NUMBER OF CREDITS	4	
NUMBER OF LECTURES PER	4	
WEEK		
TOTAL NUMBER OF LECTURES	60	
PER SEMESTER		
EVALUATION METHOD	INTERNAL	SEMESTER END
	ASSESSMENT	EXAMINATION
TOTAL MARKS	50	50
PASSING MARKS	20	20

COURSE OBJECTIVES:

CO 1.	To understand and elucidate the third law of thermodynamics and properties like
	absolute entropies, heat capacity, entropies of vaporization of liquids etc.
CO 2.	To understand and elucidate the properties of wave function, quantum operators and
	application of quantum mechanics to different systems
CO 3.	To understand the mechanism of some composite reactions, kinetics of polymerization
	reactions and theories for reaction in gas phase
CO 4.	To study Debye Huckel Onsager equation, deviations from it and to understand
	different types of fuel cells and to introduce terms, concepts and derivations involved in
	bio-electrochemistry

CLO 1.	Discuss and elucidate the Third law of thermodynamics, Trouton's rule and solve	
	problems using the properties and relationships of thermodynamic fluids	
CLO 2.	Explain and use Quantum operators in solving numericals	
CLO 3.	Understand and explain Semenov – Hinshelwood and Thompson mechanism, RRK &	
	RRKM theories	
CLO 4.	Elucidate Debye Huckel Onsager equation, Debye Falkenhagen effect, wein effect and	
	explain Bio electrochemistry concepts and derive Goldmann equation	

UNIT	THERMODYNAMICS-I	15L
1.1	State function and exact differentials. Maxwell equations, Maxwell thermodynamic Relations; it's significance and applications to ideal gases, Joule Thomson experiment, Joule Thomson coefficient, inversion temperature, Joule Thomson coefficient in terms of van der Waals constants.	8L
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. [Ref 2 and 1,10,11,12 17]	7L
UNIT	QUANTUM CHEMISTRY-I	15L
2.1	Classical Mechanics, failure of classical mechanics: Need for Quantum Mechanics.	
2.2	Particle waves and Schrödinger wave equation, wave functions, properties of wave functions, Normalization of wave functions, orthogonality of wave functions.	8L
2.3	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, Schrödinger's Time independent wave equation from Schrödinger's time dependent wave equation.	
2.4	 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. [Ref 7, 8 and 9] 	
UNIT	CHEMICAL DYNAMICS-I	15L
3.1	Composite Reactions:	
J.1	Recapitulation: Rate laws, Differential rate equations Consecutive reactions, Steady state Approximation, rate determining steps, Microscopic Reversibility and Detailed Balanced Chain reactions-chain initiation processes. Some inorganic mechanisms: formation and decomposition of phosgene, decomposition of ozone, Reaction between Hydrogen and Bromine and some general examples Organic Decompositions: Decomposition of ethane,	

	decomposition of acetaldehyde Gas phase combustion: Reaction between	
	hydrogen and oxygen, Semenov - Hinshelwood and Thompson mechanism,	
	Explosion limits and factors affecting explosion limits.	
3.2	Polymerization reactions: Kinetics of stepwise polymerization, Calculation	
	of degree of polymerization for stepwise reaction. Kinetics of free radical	
	chain polymerization, Kinetic chain length and estimation of average no .of	
	monomer units in the polymer produced by chain polymerization.	
3.3	Reaction in Gas Phase	
	Unimolecular Reactions: Lindeman-Hinshelwood theory, Rice-Ramsperger-	
	Kasssel (RRK) theory, Rice-Ramsperger-Kassel Marcus (RRKM) theory.	
	[Ref. 2 and 15, 17, 18]	
UNIT	ELECTROCHEMISTRY	15L
4		
4.1	Recapitulation – basics of electrochemistry. Debye-Hückel theory of activity	
	coefficient, Debye-Hückel limiting law and it's extension to higher	
	concentration (derivations are expected).	
	• /	
4.2	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.	
4.3	Batteries: Alkaline fuel cells, Phosphoric acid fuel cells, High temperature fuel	
	cells [Solid –Oxide Fuel Cells (SOFC) and Molten Carbonate Fuel Cells]	
4.4	Bio-electrochemistry: Introduction, cells and membranes, membrane	
	potentials, theory of membrane potentials, interfacial electron transfer in	
	biological systems, adsorption of proteins onto metals from solution, electron	
	transfer from modified metals to dissolved protein in solution, enzymes as	
	electrodes, electrochemical enzyme-catalysed oxidation of styrene.	
	Goldmann equation. (derivations are expected) [Ref: 14 and 16, 17,	
	18] [Note: Numerical and theoretical problems from each unit are	
	expected]	

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- 1. Peter Atkins and Julio de Paula, Atkin's *Physical Chemistry*, 7thEdn., Oxford University Press, 2002.
- 2. K.J. Laidler and J.H. Meiser, *Physical Chemistry*, 2nd Ed., CBS Publishers and Distributors, New Delhi, 1999.
- 3. Robert J. Silby and Robert A. Alberty, *Physical Chemistry*, 3^aEdn., John Wiley and Sons (Asia) Pte. Ltd., 2002.
- 4. Ira R. Levine, *Physical Chemistry*, 5^aEdn., Tata McGraw-Hill New Delhi, 2002.
- 5. G.W. Castellan, *Physical Chemistry*, 3rdEdn., Narosa Publishing House, New Delhi, 1983.
- 6. S. Glasstone, Text Book of Physical Chemistry, 2^MEdn., McMillan and Co. Ltd., London, 1962
- 7. B.K. Sen, *Quantum Chemistry including Spectroscopy*, Kalyani Publishers, 2003.
- 8. A.K. Chandra, Introductory Quantum Chemistry, Tata McGraw Hill, 1994.

- 9. R.K. Prasad, *QuantumChemistry*, 2ndEdn., New Age International Publishers, 2000.
- 10. S. Glasstone, Thermodynamics for Chemists, Affiliated East-West Press, New Delhi, 1964.
- 11. W.G. Davis, *Introduction to Chemical Thermodynamics A Non Calculus Approach*, Saunders, Philadelphia, 19772.
- 12. Peter A. Rock, *Chemical Thermodynamics*, University Science Books, Oxford University Press, 1983.
- 13. Ira N. Levine, *Quantum Chemistry*, 5*Edn., Pearson Education (Singapore) Pte. Ltd., Indian Branch, New Delhi, 2000.
- 14. Thomas Engel and Philip Reid, Physical Chemistry, 3dEdn., Pearson Education Limited 2013.
- 15. D.N. Bajpai, Advanced Physical Chemistry, S. Chand 1 Edn., 1992.
- 16. *Bockris*, John O'M., *Reddy*, Amulya K.N., Gamboa-Aldeco, Maria E., Modern Electrochemistry, 2A, Plenum Publishers, 1998.
- 17. Physical Chemistry by Gurtu and Gurtu
- 18. A Text book of Physical Chemistry by K L kapoorVol 5, 2ndEdn

NAME OF THE COURSE	PHYSICAL CHEMISTRY PRACTICAL	
CLASS	MSC	
COURSE CODE	SMSCHEP101	
NUMBER OF CREDITS	2	
NUMBER OF LECTURES PER	4	
WEEK		
TOTAL NUMBER OF LECTURES	60	
PER SEMESTER		
EVALUATION METHOD	INTERNAL	SEMESTER END
	ASSESSMENT	EXAMINATION
TOTAL MARKS	-	50
PASSING MARKS		20

CO 1.	To train the students in handling various instruments, glassware, chemicals etc. used in
	various analyses
CO 2.	To instruct the learner in practical knowledge on planning and performing experiments.
CO 3.	To elucidate knowledge about the non-instrumental techniques

COURSE LEARNING OUTCOMES:

The learner will be able to

CLO 1.	Follow instructions thoroughly	
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CLO 2.	Carefully handle and use various instruments used in the lab for performing	
	experiments	
CLO 3.	Perform experiments with accuracy and perfection	

PHYSICAL CHEMISTRY PRACTICAL		
Non -	Instrumental:	
2. 3. 4.	To determine the heat of solution (ΔH) of a sparingly soluble acid (benzoic /salicylic acid) from solubility measurement at three different temperature. To study the variation of calcium sulphate with ionic strength and hence determine the thermodynamic solubility product of CaSO4 at room temperature. To investigate the reaction between acetone and iodine. To study the variation in the solubility of Ca(OH)2 in presence of NaOH and hence to determine the solubility product of Ca(OH)2 at room temperature. Graph Plotting of mathematical functions –linear, exponential and trigonometry and identify whether functions are acceptable or non-acceptable	
	Instrumental:	
	 To determine the mean ionic activity coefficient of an electrolyte by e.m.f. measurement. To study the effect of substituent on the dissociation constant of acetic acid conductometrically. To determine pKa values of phosphoric acid by potentiometric titration with sodium hydroxide using glass electrode. To verify Ostwald's dilution law and to determine the dissociation constant of a weak mono-basic acid conductometrically. 	

REFERENCES:

- 1. Practical Physical Chemistry, B. Viswanathan and P.S. Raghavan, Viva Books Private Limited, 2005.
- 2. Practical Physical Chemistry, A.M. James and F.E. Prichard, 3rdEdn., Longman Group Ltd., 1974.
- 3. Experimental Physical Chemistry, V.D. Athawale and P. Mathur, New Age International Publishers, 2001.

NAME OF THE COURSE	INORGANIC CHEMIS	TRY	
CLASS	MSC		
COURSE CODE	SMSCHE102		
NUMBER OF CREDITS	4		
NUMBER OF LECTURES PER	4		
WEEK			
TOTAL NUMBER OF LECTURES	60		
PER SEMESTER			
EVALUATION METHOD	INTERNAL	SEMESTER END	
	ASSESSMENT	EXAMINATION	
TOTAL MARKS	50	50	
PASSING MARKS	20	20	

CO 1.	To understand wave functions for different hybridizations and bonding in diatomic and	
	polyatomic species	
CO 2.	To understand construction of character tables for different point groups and	
	applications of group theory	
CO 3.	To understand the methods of preparation and properties of co-ordination compounds	
	and nano particles	

CLO 1.	Derive wave functions for different hybridization and plot MOT diagrams for diatomic and polyatomic species	
CLO 2.	Construct character tables for different point groups and apply of group theory to	
	inorganic molecules	
CLO 3.	Write the methods of preparation and explain the properties of coordination	
	compounds and nanoparticles	

UNIT	CHEMICAL BONDING	15L
1		
1.1	Recapitulation of hybridization Derivation of wave functions for sp , sp^2 ,	
	sp^3 orbital hybridization types considering only sigma bonding.	
1.2	Discussion of involvement of d orbitals in various types of hybridizations.	
	Concept of resonance, resonance energy derivation expected. Formal charge	
	with examples.	
1.3	Critical analysis of VBT.	
1.4	Molecular Orbital Theory for diatomic species of First transition Series	

1.5	Molecular Orbital Theory for Polyatomic species considering σ bonding for SF ₆ , CO ₂ , B ₂ H ₆ , I ₃ molecular species.	
1.6	Weak forces of attraction: Hydrogen bonding – concept, types, properties, methods of detection and importance. Van der Waal's forces, ion-dipole, dipole-dipole, London forces.	
UNIT 2	MOLECULAR SYMMETRY AND GROUP THEORY	
2.1	Symmetry criterion of optical activity, symmetry restrictions on dipole moment. A systematic procedure for symmetry classification of molecules.	
2.2	Concepts of Groups, Sub-groups, Classes of Symmetry operations, Group Multiplication Tables. Abelian and non-Abelian point groups.	
2.3	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 ₂ v, C ₃ v and D _{2b} , structure of character tables.	
2.4	Applications of Group Theory a) Symmetry adapted linear combinations (SALC), symmetry aspects of MO theory, sigma bonding in AB _a (Ammonia, CH _a) 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. f) Descent and ascent in symmetry correlation diagrams showing relationship between different groups.	
UNIT 3	MATERIALS CHEMISTRY AND NANOMATERIALS	15L
3.1	Solid State Chemistry	
3.1.1	Electronic structure of solids and band theory, Fermi level, K Space and Brillouin Zones.	
3.1.2	Structures of Compounds of the type: AB [nickel arsenide (NiAs)], AB ₂ [fluorite (CaF ₂) and anti-fluorite structures, rutile (TiO ₂) structure and layer structure [cadmium chloride and iodide (CdCl ₂ , CdI ₂)].	
3.1.3	Methods of preparation for inorganic solids: Ceramic method, precursor method, sol-gel method (applications in Biosensors), microwave synthesis (discussion on principles, examples, merits and demerits are expected)	
3.2.1	Nanomaterials Preparative methods: Chemical methods, Solvothermal, Combustion synthesis, Microwave, Co-precipitation, Langmuir Blodgett(L-B) method, Biological methods: Synthesis using microorganisms.	
3.2.2	Applications in the field of semiconductors, solar cells	
UNIT 4	CHARACTERISATION OF COORDINATION COMPOUNDS	15L

4.1	Formation, thermal studies, Conductivity measurements, electronic spectral and magnetic measurements, IR, NMR and ESR spectroscopic methods.	
4.2	Spectral calculations using Orgel and Tanabe-Sugano diagram,	
	calculation oF electronic parameters such as Δ, Β, C,	
	Nephelauxetic ratio.	
4.3	Determination of formation constants of metal complexes (Overall and	
	Stepwise): Comparative studies of Potentiometric and spectral methods.	

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- 2. W. W. Porterfield, Inorganic Chemistry-A Unified Approach, 2nd Ed., Academic Press, 1993.
- 3. B. W. Pfennig, Principles of Inorganic Chemistry, Wiley, 2015.
- 4. C. E. Housecroft and A. G. Sharpe, Inorganic Chemistry, Pearson Education Limited, 2nd Edition 2005.
- 5. J. Huheey, F. A. Keiter and R. I. Keiter, Inorganic Chemistry–Principles of Structure and Reactivity, 4^a Ed., Harper Collins, 1993.
- 6. P. J. Durrant and B. Durrant, Introduction to Advanced Inorganic Chemistry, Oxford University Press, 1967.
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- 8. G. Miessler and D. Tarr, Inorganic Chemistry, 3rd Ed., Pearson Education, 2004.
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- 10. C. M. Day and J. Selbin, Theoretical Inorganic Chemistry, Affiliated East West Press Pvt. Ltd., 1985.
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- 12. G. A. Jeffrey, An Introduction to Hydrogen Bonding, Oxford University Press, Inc., 1997.
- 13. F. A. Cotton, Chemical Applications of Group Theory, 2nd Edition, Wiley Eastern Ltd., 1989.
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- 16. K. V. Reddy. Symmetry and Spectroscopy of Molecules, 2nd Edition, New Age International Publishers, New Delhi, 2009.
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- 20. Solid State Chemistry Introduction, Lesley E. Smart, Elaine A. Moore, ISBN 0-20349635-3, Taylor & Francis Group, LLC.
- 21. Nanomaterials&Nanochemistry, 2007, Catherine Brechignac, Philippe Houdy, Marcel Lahmani, ISBN 978-3-540-72992-1 Springer Berlin Heidelberg New York.
- 22. Nanomaterials Chemistry, Recent Developments and New Directions C.N.R. Rao, A. Muller, and A.K. Cheetham, ISBN 978-3-527-31664-9, 2007 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.
- 23. Nano-Surface Chemistry, 2001, Morton Rosoff, ISBN: 0-8247-0254-9, Marcel Dekker Inc. New York.
- 24. The Chemistry of Nanomaterials, CNR Rao, Muller Cheetham, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2004.
- 25. Semiconductor Nanomaterials, Challa S.S.R. Kumar, ISBN: 978-3-527-32166-7, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2010.
- 26. J. E. Huheey, E. A. Keiter and R. L. Keiter; Inorganic Chemistry: Principles of Structure and Reactivity, Pearson Education, 2006.
- 27. D. Banerjea , Coordination Chemistry
- 28. Geary Coordination reviews
- 29. P.W. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong; Shriver & Atkins: Inorganic Chemistry, 4th ed. Oxford University Press, 2006.
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- 31. B. Douglas, D. McDaniel and J. Alexander. *Concepts and Models of Inorganic Chemistry* (3rd edn.), John Wiley & Sons (1994).

NAME OF THE COURSE	INORGANIC CHEMISTRY PRACTICAL		
CLASS	MSC		
COURSE CODE	SMSCHEP102		
NUMBER OF CREDITS	2		
NUMBER OF LECTURES PER	4		
WEEK			
TOTAL NUMBER OF LECTURES	60		
PER SEMESTER			
EVALUATION METHOD	INTERNAL	SEMESTER END	
	ASSESSMENT	EXAMINATION	
TOTAL MARKS	-	50	
PASSING MARKS		20	

CO 1.	To train students to prepare simple nano particle	
CO 2.	To use classical methods to estimate percentage of metal in alloys/ores	
CO 3.	To use instrumental methods of analysis for estimation of metal ions and inorganic	
	compounds	

COURSE LEARNING OUTCOMES:

CLO 1.	Prepare simple nanoparticles and characterize them using absorption methods	
CLO 2.	Identify and use simple classical methods and calculate percentage composition of	
	metals in alloys/ores	
CLO 3.	Estimate metal ions and inorganic compounds using instrumental methods	

	INORGANIC CHEMISTRY PRACTICAL	
Ores	and Alloys	
1.	Analysis of Devarda's alloy	
2.	Analysis of Cu – Ni alloy	
3.	Analysis of Tin Solder alloy	
4.	Analysis of Limestone.	
Instrumentation		
1. Estimation of Copper using Iodometric method Potentiometrically.		
2. Estimation of Fe ¹³ solution using Ce(IV) ions Potentiometrically		

REFERENCE:

- 1. Advanced experiments in Inorganic Chemistry., G. N. Mukherjee., 1 Edn., 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: <u>Dr Deepak Pant</u>

NAME OF THE COURSE	ORGANIC CHEMISTRY
CLASS	MSC
COURSE CODE	SMSCHE103
NUMBER OF CREDITS	4
NUMBER OF LECTURES PER	4
WEEK	
TOTAL NUMBER OF LECTURES	60

PER SEMESTER		
EVALUATION METHOD	INTERNAL	SEMESTER END
	ASSESSMENT	EXAMINATION
TOTAL MARKS	50	50
PASSING MARKS	20	20

CO 1.	Understand the mechanisms of reactions and the effect of various parameters on the	
CO 1.	1	
	rate of the reaction, stereochemistry and selectivity of the product.	
CO 2.	Understand the criteria of aromaticity, thermochemical and magnetic criteria for	
	aromatic compounds of benzenoid and non-benzenoid structures and earn to draw the	
	Frost Musulin Diagrams for various compounds.	
CO 3. Understand the stereochemical concepts in molecules with constitutionally		
	and asymmetric stereoisomers, the principles of axial and planar chirality, the	
	configurational descriptors to allenes, alkylidene cycloalkanes, spirans, biaryls	
	(including BINOLs and BINAPs), ansa compounds, cyclophanes, the concepts of	
	topicity, criteria for enantiotopic and disastereotopic ligands and faces and identify	
	them in a stereoisomer.	
CO 4.	Understand how to assign configurational descriptors for enantiotopic and	
	diastereotopic faces and the concept of prochirality and predicting them in a molecule	
İ		

CLO 1. Students are expected to predict a mechanism, rate of the reaction, stereochemical outcome of reactions, understanding the factors affecting acidity and basicity and involvement of acids and bases in determining the mechanism. CLO 2. Predicting the stereochemical concepts in molecules with constitutionally symmetric and asymmetric stereoisomers, applying the principles of axial and planar chirality. assigning configurational descriptors to allenes, alkylidene cycloalkanes, spirans, biaryls (including BINOLs and BINAPs), ansa compounds, cyclophanes, Predicting topicity, evaluating the criteria for enantiotopic and disastereotopic ligands
CLO 2. Predicting the stereochemical concepts in molecules with constitutionally symmetric and asymmetric stereoisomers, applying the principles of axial and planar chirality. assigning configurational descriptors to allenes, alkylidene cycloalkanes, spirans, biaryls (including BINOLs and BINAPs), ansa compounds, cyclophanes,
and asymmetric stereoisomers, applying the principles of axial and planar chirality. assigning configurational descriptors to allenes, alkylidene cycloalkanes, spirans, biaryls (including BINOLs and BINAPs), ansa compounds, cyclophanes,
assigning configurational descriptors to allenes, alkylidene cycloalkanes, spirans, biaryls (including BINOLs and BINAPs), ansa compounds, cyclophanes,
biaryls (including BINOLs and BINAPs), ansa compounds, cyclophanes,
Predicting topicity, evaluating the criteria for enantiotopic and disastereotopic ligands
and faces and identifying them in a stereoisomer and assigning configurational
descriptors Identifying a prochiral center and assigning descriptors.
CLO 3. Classify the compounds based on criteria of aromaticity, analyse the thermochemical
and magnetic data for aromatic compounds of benzenoid and non-benzenoid structure
and drawing frost musulin diagrams
CLO 4. Predicting Selectivity and specificity of the various oxidizing and reducing reagents
and the mechanism and identifying suitable reagents required for designing synthesis
via functional group interconversion.

UNIT 1	PHYSICAL ORGANIC CHEMISTRY	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	Determining mechanism of a reaction: Product analysis, kinetic studies, use of isotopes (Kinetic isotope effect – primary and secondary kinetic isotope effect). Detection and trapping of intermediates, crossover experiments and stereochemical evidence.	
1.3	Acids and Bases: Factors affecting acidity and basicity: Electronegativity and inductive effect, resonance, bond strength, electrostatic effects, hybridization, aromaticity and solvation. Comparative study of acidity and basicity of organic compounds on the basis of pKa values, Leveling effect and non-aqueous solvents. Acid and base catalysis – general and specific catalysis with examples. [Reference Books: 1, 2, 3, 16]	
UNIT 2	NUCLEOPHILIC SUBSTITUTION REACTIONS AND AROMATICITY	15L
2.1 2.1.1	Nucleophilic substitution: S _N 1, S _N 2, S _N reactions, mixed S _N 1 and S _N 2 and SET mechanisms. S _N reactions involving NGP - participation by aryl rings, αand pi-bonds. Factors affecting these reactions: substrate, nucleophilicity, solvent, steric effect, hard-soft interaction, leaving group. Ambident nucleophiles. S _N CA, S _N 1' and S _N 2' reactions. S _N at sp ² (vinylic) carbon.	9L
2.1.2	Aromatic nucleophilic substitution: S_NAr , S_N1 , benzyne mechanisms. Ipso, cine, tele and vicarious substitution.	
2.1.3	Ester hydrolysis: Classification, nomenclature and study of all eight mechanisms of acid and base catalyzed hydrolysis with suitable examples.	
2.2 2.2.1	2.2. Aromaticity: (6 L) Structural, thermochemical, and magnetic criteria for aromaticity, including NMR characteristics of aromatic systems. Delocalization and aromaticity.	
2.2.2	Application of HMO theory to monocyclic conjugated systems. Frost-Musulin diagrams. Huckel's (4n+2) and 4n rules.	
2.2.3	Aromatic and antiaromatic compounds up-to 18 carbon atoms. Homoaromatic compounds. Aromaticity of all benzenoid systems, heterocycles, metallocenes, azulenes, annulenes, aromatic ions and	

	Fullerene (C ₆₀). [Reference Books: 4-15]	
UNIT	STEREOCHEMISTRY	
3		
3.1	Concept of Chirality: Recognition of symmetry elements.	
3.2	Molecules with tri- and tetra-coordinate centers: Compounds with	
	carbon, silicon, nitrogen, phosphorous and sulphur chiral centers, relative configurational stabilities.	
3.3	Molecules with two or more chiral centers: Constitutionally unsymmetrical molecules: erythro-threo and syn-anti systems of nomenclature. Interconversion of Fischer, Sawhorse, Newman and Flying wedge projections. Constitutionally symmetrical molecules with odd and even number of chiral centers: enantiomeric and meso forms, concept of stereogenic, chirotopic, and pseudoasymmetriccentres. R-S nomenclature for chiral centres in acyclic and cyclic compounds.	
3.4	Axial and planar chirality: Principles of axial and planar chirality. 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, trans-cyclooctenes.	
3.5	Prochirality: Chiral and prochiralcentres; prochiral axis and prochiral plane. Homotopic, heterotopic (enantiotopic and diastereotopic) ligands and faces. Identification using substitution and symmetry criteria. Nomenclature of stereoheterotopic ligands and faces. Symbols for stereoheterotopic ligands in molecules with i) one or more prochiralcentres ii) a chiral as well as a prochiralcentre, iii) a prochiral axis iv) a prochiral plane v) propseudoasymmetriccentre. Symbols for enantiotopic and diastereotopic faces. [Reference Books: 6-8]	
TINITE	[Reference Books: 6-8]	4.57
UNIT 4	OXIDATION AND REDUCTION	15L
4.1	Oxidation: General mechanism, selectivity, and important applications of the following:	
4.1.1	Dehydrogenation: Dehydrogenation of C-C bonds including aromatization of six membered rings using metal (Pt, Pd, Ni) and organic reagents (chloranil, DDQ)	
4.1.2	Oxidation of alcohols to aldehydes and ketones: Chromium reagents such as K ₂ Cr ₂ O ₇ /H ₂ SO ₄ (Jones reagent), CrO ₃ -pyridine (Collin's reagent), PCC (Corey's reagent) and PDC (Cornforth reagent), hypervalent iodine reagents (IBX, Dess-Martin periodinane). DMSO based reagents (Swern oxidation), Corey-Kim oxidation - advantages over Swern and limitations;	

	and Pfitzner-Moffatt oxidation-DCC and DMSO and Oppenauer oxidation.	
4.1.3	Oxidation involving C-C bonds cleavage: Glycols using HIO.; cycloalkanones using CrO.; carbon-carbon double bond using ozone, KMnO., CrO., NaIO., and OsO.; aromatic rings using RuO., and NaIO.	
4.1.4	Oxidation involving replacement of hydrogen by oxygen: oxidation of CH ₂ to CO by SeO ₂ , oxidation of arylmethanes by CrO ₂ Cl ₂ (Etard oxidation).	
4.1.5	Oxidation of aldehydes and ketones: with H ₂ O ₂ (Dakin reaction), with peroxy acid (Baeyer-Villiger oxidation)	
4.2	Reduction: General mechanism, selectivity, and important applications of the following reducing reagents:	
4.2.1	Reduction of CO to CH ₂ in aldehydes and ketones-Clemmensen reduction, WolffKishner reduction and Huang-Minlon modification.	
4.2.2	Metal hydride reduction: Boron reagents (NaBH ₄ , NaCNBH ₃ , diborane, 9-BBN, Na(OAc) ₃ BH, aluminium reagents (LiAlH ₄ , DIBAL-H, Red Al, L and K-selectrides).	
4.2.3	NH ₂ NH ₂ (diimide reduction) and other non-metal based agents including organic reducing agents (Hantzschdihydropyridine).	
4.2.4	Dissolving metal reductions: using Zn, Li, Na, and Mg under neutral and acidic conditions, Li/Na-liquid NH, mediated reduction (Birch reduction) of aromatic compounds and acetylenes. [Reference Books: 17, 18, 14]	

REFERNCES

- 1. Physical Organic Chemistry, Neil Isaacs
- 2. Modern Physical Organic Chemistry, Eric V. Anslyn and Dennis A. Dougherty
- 3. Comprehensive Organic chemistry, Barton and Ollis, Vol 1
- 4. Organic Chemistry, J. Claydens, N. Greeves, S. Warren and P. Wothers, Oxford University Press.
- 5. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Part A and B, Plenum Press.
- 6. Stereochemistry: Conformation and mechanism, P.S. Kalsi, New Age International, New Delhi.
- 7. Stereochemistry of carbon compounds, E.L Eliel, S.H Wilen and L.N Manden, Wiley.
- 8. Stereochemistry of Organic Compounds- Principles and Applications, D. Nasipuri. New International Publishers Ltd.
- 9. March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, Michael B. Smith, Jerry March, Wiley.
- 10. Advanced Organic Chemistry: Reactions and mechanism, B. Miller and R. Prasad, Pearson Education.
- 11. Advanced Organic Chemistry: Reaction mechanisms, R. Bruckner, Academic Press.
- 12. Understanding Organic Reaction Mechanisms, Adams Jacobs, Cambridge University Press.
- 13. Writing Reaction Mechanism in organic chemistry, A. Miller, P.H. Solomons, Academic Press.
- 14. Principles of Organic Synthesis, R.O.C. Norman and J.M Coxon, Nelson Thornes.

- 15. Advanced Organic Chemistry: Reactions and mechanism, L.G. Wade, Jr., Maya Shankar Singh, Pearson Education.
- 16. Mechanism in Organic Chemistry, Peter sykes, 6th edition onwards.
- 17. Modern Methods of Organic Synthesis, W. Carruthers and Iain Coldham, Cambridge University Press.
- 18. Organic Synthesis, Jagdamba Singh, L.D.S. Yadav, PragatiPrakashan.

ORGANIC CHEMISTRY PRACTICAL		
MSC		
SMSCHEP103	SMSCHEP103	
2		
4		
60		
INTERNAL	SEMESTER END	
ASSESSMENT	EXAMINATION	
-	50	
	20	
	MSC SMSCHEP103 2 4 60 INTERNAL	

Learners will learn to:

CO 1.	To synthesize organic compounds.
CO 2.	To purify the given compound by suitable method
CO 3.	Techniques of TLC to study the progress of a reaction

CLO 1.	Prepare organic compounds at micro scale
CLO 2.	To assess the purity of the prepared compound
CLO 3.	Monitor the progress of the reaction using TLC

ORGANIC CHEMISTRY PRACTICAL	
One step preparations (1.0 g scale)	
1. Bromobenzene to p-nitrobromobenzene	
2. Anthracene to anthraquinone	
3. Benzoin to benzil	

- 4. Anthracene to Anthracene maleic anhydride adduct
- 5. 2-Naphthol to BINOL
- 6. p-Benzoquinone to 1,2,4-triacetoxybenzene
- 7. Ethyl acetoacetate to 3-methyl-1-phenylpyrazol-5-one
- 8. o-Phenylenediamine to 2-methylbenzimidazole
- 9. o-Phenylenediamine to 2,3-diphenylqunooxaline
- 10. Urea and benzil to 5,5-diphenylhydantoin

Learning points:

- 1. Planning of synthesis, effect of reaction parameters including stoichiometry, and safety aspects including MSDS should be learnt.
- 2. Purify the product by crystallization. Formation and purity of the product should be checked by TLC
- 3. Report mass and melting point of the purified product.

NAME OF THE COURSE	ANALYTICAL CHEMISTRY	
CLASS	MSC	
COURSE CODE	SMSCHE104	
NUMBER OF CREDITS	4	
NUMBER OF LECTURES PER	4	
WEEK		
TOTAL NUMBER OF LECTURES	60	
PER SEMESTER		
EVALUATION METHOD	INTERNAL	SEMESTER END
	ASSESSMENT	EXAMINATION
TOTAL MARKS	50	50
PASSING MARKS	20	20

COURSE OBJECTIVES:

CO 1.	To introduce important terms involved in analytical chemistry and to create awareness	
	about quality, accreditation and GLP	
CO 2.	To learn and use appropriate concentration units and predict yield of a reaction.	
CO 3.	To learn about FTIR and UV-Vis spectroscopy as an analytical tool.	
CO 4.	To learn about DSC, DTA and thermometric titration methods as a method for the	
	characterisation of various substances.	

COURSE LEARNING OUTCOMES:

The learner will be able to

CLO 1.	Understand the use and importance of various terms used in analytical chemistry and	
	Comprehend various quality standards and safety rules followed in the laboratories	
CLO2.	Interconvert various concentration units and assess conditions to improve reaction	
	yield.	
CLO 3.	Explain the working and applications of IR, FTIR and UV-Vis spectroscopy in various	
	fields	
CLO4	To solve numerical problems on simultaneous spectroscopy.	
	interpret thermograms of various compounds for identification and quantification.	

UNIT 1	LANGUAGE OF AND QUALITY IN ANALYTICAL CHEMISTRY	
1.1	Language of Analytical chemistry	9L
1.1.1	Analytical perspective, Common analytical problems, terms involved in analytical chemistry (analysis, determination, measurement, techniques, methods, procedures and protocol)	
1.1.2	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.	
1.1.3	Errors, determinate and indeterminate errors. Types of determinate errors, tackling of errors.	
1.1.4 4	Quantitative methods of analysis: calibration curve, standard addition and internal standard method.	
1.2	Quality in Analytical Chemistry:	7L
1.2.1	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.	
1.2.2.	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).	
1.2.3	Accreditations: Accreditation of Laboratories, Introduction to ISO series, Indian Government Standards (ISI, Hallmark, Agmark)	
1.2.4	Good Laboratory Practices (GLP) Principle, Objective, OECD guidelines, The US FDA 21CFR58, Klimisch score	

UNIT 2	CALCULATIONS BASED ON CHEMICAL PRINCIPLES			
	The following topics are to be covered in the form of numerical problems only.			
	a) Concentration of a solution based on volume and mass units.			
	b) Calculations of ppm, ppb and dilution of the solutions, concept of mmol.			
	c) Stoichiometry of chemical reactions, concept of kg mol, limiting reactant, theoretical and practical yield.			
	d) Solubility and solubility equilibria, effect of presence of common ion.			
	e) Calculations of pH of acids, bases, acidic and basic buffers.			
	f) Concept of formation constants, stability and instability constants, stepwise formation constants.			
	g) 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).			
UNIT 3	OPTICAL METHODS	15L		
3.1	Recapitulation and FT Technique	3L		
	Recapitulation of basic concepts, Electromagnetic spectrum, Sources, Detectors, sample containers.			
	a) Laser as a source of radiation, Fibre optics			
	b) Introduction of Fourier Transform			
3.2	Molecular Ultraviolet and Visible Spectroscopy NUMERICALS ARE EXPECTED			
3.2.1 Do	erivation of Beer- Lambert's Law and its limitations, 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:			
	a) On charge transfer absorptionb) Simultaneous spectroscopyc) Derivative Spectroscopy			
3.2.2	Dual spectrometry – Introduction, Principle, Instrumentation and Applications			

	Instrumentation: Sources, Sample handling, Transducers, Dispersive, non-dispersive instrument	
	a) FTIR and its advantages	
	b) Applications of IR [Mid IR, Near IR, Far IR]: Qualitative with emphasis on "Finger print" region, Quantitative analysis, Advantages and Limitations of IR	
	c) Introduction and basic principles of diffuse reflectance spectroscopy.	
UNIT	THERMAL METHODS	
4		
4.1	Thermal Methods:	9 L
4.1.1	Introduction, Recapitulation of types of thermal methods, comparison	
	between TGA and DTA.	
4.1.2	Differential Scanning Calorimetry- Principle, comparison of DTA and	
	DSC, Instrumentation, Block diagram, Nature of DSC Curve, Factors	
	affecting curves (sample size, sample shape, pressure).	
4.1.3	Applications - Heat of reaction, Specific heat, Safety screening, Polymers, liquid crystals, Percentage cystallinity, oxidative stability, Drug analysis, Magnetic transition. e.g. Analysis of Polyethylene for its crystallinity.	
4.2	Automation in chemical analysis:	6 L
	Need for automation, Objectives of automation, An overview of automated instruments and instrumentation, process control analysis, flow injection analysis, discrete automated systems, automatic analysis based on multilayered films, gas monitoring equipments, Automatic titrators.	

REFERNCES:

- 1. Modern Analytical Chemistry by David Harvey, McGraw-Hill Higher Education Principles of Instrumental Analysis Skoog, Holler and Nieman, 5^a Edition, Ch:
- 2. Fundamentals of Analytical Chemistry, By Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, 9th Edition, 2004, Ch: 5.
- 3. Undergraduate Instrumental Analysis, 6th Edition, J W Robinson, Marcel Dekker, Ch:1.
- 4. ISO 9000 Quality Systems Handbook, Fourth Edition, David Hoyle. (Chapter: 3 & 4) (Free download).
- 5. Quality in the Analytical Laboratory, Elizabeth Pichard, Wiley India, Ch. 5, Ch. 6 & Ch. 7.
- 6. Quality Management, Donna C S Summers, Prentice-Hall of India, Ch:3.
- 7. Quality in Totality: A Manager's Guide To TQM and ISO 9000, ParagDiwan, Deep & Deep Publications, 1st Edition, 2000.
- 8. Quality Control and Total Quality Management P.L. Jain-Tata McGraw-Hill (2006) Total Quality Management Bester field Pearson Education, Ch:5.

- 9. Industrial Hygiene and Chemical Safety, M H Fulekar, Ch:9, Ch:11 & Ch:15.
- 10. Safety and Hazards Management in Chemical Industries, M N Vyas, Atlantic Publisher, Ch:4, Ch:5 & Ch:19.
- 11. Staff, World Health Organization (2009) Handbook: Good Laboratory Practice (GLP)
- 12. OECD Principles of Good Laboratory Practice (as revised in 1997)". OECD Environmental Health and Safety Publications. OECD. 1. 1998.
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- 1.3000 solved problems in chemistry, Schaums Solved problem series, David E. Goldbers, McGraw Hill international Editions, Chapter 11,15,16,21,22

Unit III

- 1. D. A. Skoog, F. J. Holler, T. A. Nieman, Principles of Instrumental Analysis, 5th Edition, Harcourt Asia Publisher. Chapter 6, 7.
- 2. H. H. Willard, L. L. Merritt, J. A. Dean, F. A. Settle, Instrumental Methods of Analysis,6 th Edition, CBS Publisher. Chapter 2.
- 3. R. D. Braun, Introduction to Instrumental Analysis, McGraw Hill Publisher. Chapter 8.
- 4. D. A. Skoog, F. J. Holler, T. A. Nieman, Principles of Instrumental Analysis, 5 th Edition, Harcourt Asia Publisher. Chapter 13, 14.
- 5. H. H. Willard, L. L. Merritt, J. A. Dean, F. A. Settle, Instrumental Methods of Analysis,6 th Edition, CBS Publisher. Chapter 2.
- 6. R. D. Braun, Introduction to Instrumental Analysis, McGraw Hill Publisher. Chapter 5.
- 7. G. W. Ewing, Instrumental Methods of Chemical Analysis, 5 th Edition, McGraw Hill Publisher, Chapter 3.
- 8. M. Ito, The effect of temperature on ultraviolet absorption spectra and its relation to hydrogen bonding, J. Mol. Spectrosc. 4 (1960) 106-124.
- 9. A. J. Somnessa, The effect of temperature on the visible absorption band of iodine inseveral solvents, Spectrochim. Acta. Part A: Molecular Spectroscopy, 33 (1977) 525528.
- 10. D. A. Skoog, F. J. Holler, T. A. Nieman, Principles of Instrumental Analysis, 5 th Edition, Harcourt Asia Publisher. Chapter 16, 17.
- 11. R. D. Braun, Introduction to Instrumental Analysis, McGraw Hill Publisher. Chapter 12
- 12. Z. M. Khoshhesab (2012). Infrared Spectroscopy- Materials Science, Engineering and Technology. Prof. TheophanidesTheophile (Ed.). ISBN: 978-953- 51-0537- 4, InTech,(open access)

Unit IV

- 1. Introduction to instrumental methods of analysis by Robert D. Braun, Mc. Graw Hill (1987): Chapter 27
- 2. 2. Thermal Analysis-theory and applications by R. T. Sane, Ghadge, Quest Publications
- 3. Instrumental methods of analysis, 7 th Edition, Willard, Merrit, Dean: Chapter 25
- 4. Instrumental Analysis, 5 th Edition, Skoog, Holler and Nieman: Chapter 31
- 5. Quantitative Chemical Analysis, 6 th Edition, Vogel: Chapter 12
- 6. Analytical Chemistry by Open Learning: Thermal Methods by James W. Dodd & Dodd & H. Tonge
- 7. Instrumental methods of analysis, 7 th Edition, Willard, Merrit, Dean: Chapter 26

- 8. Instrumental Analysis, 5th Edition, Skoog, Holler and Nieman: Chapter 33
- 9. Introduction to instrumental methods of analysis by Robert D. Braun, Mc. GrawHill (1987): Chapter 28

	I	
NAME OF THE COURSE	ANALYTICAL CHEMISTRY PRACTICAL	
CLASS	MSC	
COURSE CODE	SMSCHEP104	
NUMBER OF CREDITS	2	
NUMBER OF LECTURES PER	4	
WEEK		
TOTAL NUMBER OF LECTURES	60	
PER SEMESTER		
EVALUATION METHOD	INTERNAL	SEMESTER END
	ASSESSMENT	EXAMINATION
TOTAL MARKS	-	50
PASSING MARKS		20

CO 1.	To learn analysis of individual and mixture of components by classical and
	instrumental methods learnt in theory.
CO 2.	To learn the role of different solvents in sample pre-treatment to enhance accuracy of
	the result
CO 3.	To get highly reproducible and accurate results irrespective of the origin of
	the sample.

COURSE LEARNING OUTCOMES:

The learner will be able to

CLO 1.	Use concepts learnt in theory for solving practical problems.
CLO 2.	Understand and apply the knowledge acquired in theory to different types of samples for its characterisation and estimation.
CLO 3.	Be able to work comfortably at different concentrations with the highest degree of accuracy and reproducibility.

ANALYTICAL CHEMISTRY PRACTICAL	
1. To carry out assay of the sodium chloride injection by Volhard's	
method.	
Statistical method.	
2. To determine (a) the ion exchange capacity (b) exchange efficiency of	
the given cation exchange resin.	

- 3. To determine amount of Cr(III) and Fe(II) individually in a mixture of the two by titration with EDTA.
- 4. To determine the breakthrough capacity of a cation exchange resin.
- 5. To determine the lead and tin content of a solder alloy by titration with EDTA.
- 6. To determine amount of Cu(II) present in the given solution containing a mixture of Cu(II) and Fe(II).
- 7. To determine number of nitro groups in the given compound using TiCl₃.

References:

- 1. Quantitative Inorganic Analysis including Elementary Instrumental Analysis by A. I. Vogels, 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. Standard Instrumental methods of Chemical Analysis, F. J. Welcher
- 5. W.W.Scott."Standard methods of Chemical Analysis", Vol.I, Van Nostrand Company, Inc., 1939.
- 6. E.B.Sandell and H.Onishi,"Spectrophotometric Determination of Traces of Metals",PartII,4thEd.,A Wiley IntersciencePublication,New York,1978.

SEMESTER II

NAME OF THE COURSE	PHYSICAL CHEMISTRY	
CLASS	MSC	
COURSE CODE	SMSCHE102	
NUMBER OF CREDITS	4	
NUMBER OF LECTURES PER	4	
WEEK		
TOTAL NUMBER OF LECTURES	60	
PER SEMESTER		
EVALUATION METHOD	INTERNAL	SEMESTER END
	ASSESSMENT	EXAMINATION
TOTAL MARKS	50	50
PASSING MARKS	20	20

COURSE OBJECTIVES:

CO 1.	To understand the concept of fugacity, Gibbs energy of mixing, relation of partial
	molal quantity with thermodynamic properties
CO 2.	To understand thermodynamics of surfaces and free energy changes of biochemical
	reactions and different types and thermodynamics of formation of defects
CO 3.	To emanate schrodinger equation in spherical coordinates, quantization of rotational
	energy and spherical harmonics, total wave functions, probability density functions and
	interdependence of quantum numbers
CO 4.	To summarize phase equilibria for two component and three component systems
	To learn kinetics of enzyme catalyzed reactions, different types of inhibitions of
	enzymes and kinetics of reactions in solid state.

CLO 1.	Deduce fugacity of real gases using graphical methods and elucidate Laplace, Kelvin equation and derive Gibbs adsorption isotherm and BET isotherm
CLO 2.	Understand and explain two particle problems and separation of variables, expressions
	for the total wave function for 1s, 2s, 2p and 3d orbitals of hydrogen.
CLO 3.	Elaborate the general mechanisms of acid-base catalysis, enzyme catalysis and effect of
	pH & temperature on them.
CLO 4.	Extrapolate mathematical equation to find concentration of defects and solve numerical
	problems based on it and Understand and explain two component systems and three
	component systems.

UNIT	THERMODYNAMICS-II	15L
1		
1.1	Fugacity of real gases - Determination of fugacity of real gases using	
	graphical method and from equation of state. Equilibrium constant for real	
	gases in terms of fugacity. Gibbs energy of mixing, entropy and enthalpy of mixing.	
1.2	Real solutions- Partial molal quantities, partial molal volume, Gibbs Duhem equation, Relation of partial molal quantity to thermodynamic properties, chemical potential in non-ideal solutions, Gibbs Duhem Margules equation.	
1.3	Thermodynamics of surfaces- Pressure difference across curved surfaces (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, BET isotherm (derivations expected).	
1.4	Bioenergetics: standard free energy change in biochemical reactions, exergonic, endergonic. Hydrolysis of ATP, synthesis of ATP from ADP.	
UNIT 2	QUANTUM CHEMISTRY-II	15L
2.1	Rigid rotor, spherical coordinates Schrödinger wave equation in spherical coordinates, separation of the variables, the phi equation, wave function, quantum number, the theta equation, wave function, quantization of rotational energy, spherical harmonics.	

2,2	Hydrogen atom, the two particle problem, separation of the energy as	8L
	translational and potential, separation of variables, the R the θ * and the ϕ	
	equations, solution of the equation, introduction of the four quantum numbers	
	and their interdependence on the basis of the solutions of the three equations,	
	total wave function, expression for the energy, probability density function,	
	distances and energies in atomic units, radial and angular plots., points of	
	maximum probability, expressions for the total wave function for 1s,2s, 2p and	
	3d orbitals of hydrogen.	
2.3	Application of the Schrödinger equation to two electron systems, limitations	
	of the equation, need for the approximate solutions, methods of obtaining the	
	approximate solution of the Schrödinger wave equation.	
2.4	Hückel Molecular Orbitals theory for ethylene, 1,3-butadiene and benzene.	
	(Derivation expected)	
UNIT	CHEMICAL DYNAMICS-II	15L
3		
2.1	Conseq Contact Made views For Elizabeth Anna to the state	
3.1	General Catalytic Mechanisms – Equilibrium treatment, steady state treatment,	
	Activation energies for catalyzed reactions	
2.2	Acid base Catalysis – general, theory and mechanism	
3.2	Kinetics of reactions catalyzed by enzymes – Michaelis - Menten analysis,	
	Lineweaver- Burk and Eadie Analyses, influence of pH and temperature.	
3.3	Inhibition of Enzyme action: Competitive, Noncompetitive and Uncompetitive	
	Inhibition. Effect of pH, Enzyme activation by metal ions, Regulatory enzymes.	
3.4	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)	
UNIT	SOLID STATE CHEMISTRY AND PHASE EQUILIBRIA	15L
4	SOLID STATE CHEMISTRY AND THASE EQUILIBRIA	131
	Call Charle Characteris	
4.1	Solid State Chemistry	
	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 and 19)	
	(101. 17, 10 dhd17)	
4.2	Phase Equilibria	
4.2.1	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)	
4.2.2	B] Three component system:	
	I. Formation of two pair of partially miscible	
	II. Formation of three pair of partially miscible liquid.	
	1 22. 2 2222 and of an or barriary importate rights.	l .
	III. Solid liquid Equilibria - Ternary solutions with common ions – (NaCl –	

KCl-H₂O and NaCl- Na₄SO₄- H₂O) (Ref: 4, 6, 11, 12, 13, 16, 24)

REFERENCES:

- 1. Peter Atkins and Julio de Paula, Atkin's Physical Chemistry, 7th Edition, Oxford University Press, 2002.
- 2. K.J. Laidler and J.H. Meiser, Physical Chemistry, 2nd Edition., CBS Publishers and Distributors, New Delhi, 1999.
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- 4. Ira R. Levine, Physical Chemistry, 5th Edition, Tata McGraw-Hill New Delhi, 2002.
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- 6. Principles of Chemical Kinetics, 2nd Ed., James E. House, ELSEVIER, 2007.
- 7. B.K. Sen, Quantum Chemistry including Spectroscopy, Kalyani Publishers, 2003.
- 8. S. Glasstone, Thermodynamics for Chemists, Affiliated East-West Press, New Delhi, 1964.
- 9. W.G. Davis, Introduction to Chemical Thermodynamics A Non Calculus Approach, Saunders, Philadelphia, 19772.
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- 11. Thomas Engel and Philip Reid, Physical Chemistry, 3rd Edition, Pearson Education Limited 2013.
- 12. Solid State Chemistry [An Introduction], 3rd Ed., Lesley E. Smart & Elaine A. Moore, Taylor & Francis, 2010.
- 13. The Physics and 'Chemistry of Solids, Stephen Elliott, Willey India, 2010
- 14. Solid State Chemistry, D.K. Chakrabarty, New Age International Publishers, 1996.
- 15. Principles of physical Chemistry, Marrown and Prutton 5th edition
- 16. Essentials of Physical Chemistry ArunBahl, B. S Bahl, G. D.Tulli, S Chand and Co. Ltd, 2012 Edition.
- 17. Introduction of Solids L.V Azaroff, Tata McGraw Hill.
- 18. A Textbook of physical Chemistry; Applications of thermodynamics vol III, Mac Millan Publishers India Ltd ,2011

NAME OF THE COURSE	PHYSICAL CHEMISTRY PRACTICAL
CLASS	MSC
COURSE CODE	SMSCHEP203
NUMBER OF CREDITS	2
NUMBER OF LECTURES PER	4
WEEK	
TOTAL NUMBER OF LECTURES	60
PER SEMESTER	

EVALUATION METHOD	INTERNAL	SEMESTER END
	ASSESSMENT	EXAMINATION
TOTAL MARKS	-	50
PASSING MARKS		20

CO 1.	To train the students in handling various instruments.
CO 2.	To get practical knowledge on planning and performing experiments
CO 3.	To gain knowledge about the non-instrumental techniques
CO 4.	To solve equations mathematically to plot graphs and interpret them.

COURSE LEARNING OUTCOMES:

The learner will be able to

CLO 1.	Be equipped with technical skills to work with various instruments.
CLO 2.	Correlate the theoretical knowledge with the practical experiments.
CLO 3.	Mathematically solve equations and Interpret graphical plots.

PHYSICAL CHEMISTRY PRACTICAL	
Non – instrumental:	
1. Study the variation of calcium sulphate with ionic strength and hence	
determine the thermodynamic solubility product of CaSO4 at room temperature.	
2. Study the influence of ionic strength on the base catalyzed hydrolysis of ethyl acetate	
3. Determine the rate constant of decomposition reaction of diacetone alcohol by dilatometric method.	
4. Polar plots of atomic orbitals such as 1s, pz and 3dz ² orbitals 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.	
3. Determine hydrolysis constant for aniline hydrochloride using conductivity measurements	
4. Determine the Michaelis – Menten's constant value (Km) of the enzyme Beta Amylase spectrophotometrically.	

REFERENCES:

- 1. Practical Physical Chemistry, B. Viswanathan and P.S. Raghavan, Viva Books Private Limited, 2005.
- 2. Practical Physical Chemistry, A.M. James and F.E. Prichard, 3rd Edition Longman Group Ltd., 1974.
- 3. Experimental Physical Chemistry, V.D. Athawale and P. Mathur, New Age International Publishers, 2001.

NAME OF THE COURSE	INORGANIC CHEMIS	TRY
CLASS	MSC	
COURSE CODE	SMSCHE202	
NUMBER OF CREDITS	4	
NUMBER OF LECTURES PER	4	
WEEK		
TOTAL NUMBER OF LECTURES	60	
PER SEMESTER		
EVALUATION METHOD	INTERNAL	SEMESTER END
	ASSESSMENT	EXAMINATION
TOTAL MARKS	50	50
PASSING MARKS	20	20

CO 1.	To understand different types of reactions and their mechanisms for inorganic
	complexes of varying geometry.
CO 2.	To impart knowledge of sources, effects, control measures of radioactive pollutants and
	heavy metals.
CO 3.	To understand the role of metals in biological systems

COURSE LEARNING OUTCOMES:

The learner will be able to:

CLO 1.	Identify different types of reactions and their mechanisms for inorganic complexes of
	varying geometry
CLO 2.	Suggest methods for environmental protection and explain effects of radiation and
	heavy metal
CLO 3.	Explain the role of metals in biological systems

UNIT 1	INORGANIC REACTION MECHANISM	15L
1.1	Rate of reactions, factors affecting the rate of reactions, techniques for determination of rate of reaction (Direct chemical analysis, spectrophotometric	3L

	method, electrochemical and flow methods).	
1.2	Ligand substitution reactions of: (Mechanism and factors affecting these substitution reactions.)	5L
	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	
1.3	Redox reactions: electron and atom transfer, inner and outer sphere	4L
	mechanisms, complimentary and non-complimentary reactions.	
1.4	Stereochemistry of substitution reactions of octahedral complexes.	3L
	(Isomerization and racemization reactions and applications.)	
UNIT	ORGANOMETALLIC CHEMISTRY OF TRANSITION METALS	15L
2		
2.1	Eighteen and sixteen electron rule comparison and electron counting with	2L
	examples.	
2.2	Preparation and properties of the following compounds	10L
	(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.	
2.3	Structure and bonding on the basis of VBT and MOT in the following	3L
	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).	
UNIT	ENVIRONMENTAL CHEMISTRY	15L
3		102
3.1	Introduction and discussion of toxicity of Heavy Metals: Toxicity of metallic	5 L
	species: Mercury, lead, cadmium, arsenic, copper and chromium, with respect	
	to their sources, distribution, speciation, biochemical effects and toxicology, control and treatment.	
3.2	Case Studies: For example	5L
- ·-	(a) Itai-itai disease for Cadmium toxicity,	
	(b) Arsenic Poisoning in the Indo-Bangladesh region.	
	(Other relevant examples recent may be included)	
3.3	Interaction of radiation in context with the environment:Sources and	5L
	biological implication of radioactive materials. Effect of low level radiation	
	on cells- Its applications in diagnosis and treatment, Effect of radiation on	
	cell proliferation and cancer.	
UNIT	BIOINORGANIC CHEMISTRY	15L
4		
4.1	Biological oxygen carriers- heme and non heme: hemoglobin, hemerythrene and hemocyanin- structure of metal active center and differences in	7L

	mechanism of oxygen binding, Differences between hemoglobin and myoglobin: Cooperativity of oxygen binding in hemoglobin and Hill equation, pH dependence of oxygen affinity in hemoglobin and myoglobin and its implications.	
4.2	Copper containing enzymes- superoxide dismutase, tyrosinase and laccase: catalytic reactions and the structures of the metal binding site	3L
4.3	Nitrogen fixation-nitrogenase, hydrogenases	3L
4.4	Metal ion transport and storage: Ionophores and metallothionins	2L

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- 1. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Inorganic Chemistry, 5th Ed., Oxford University Press, 2010.
- 2. W. H. Malik, G. D. Tuli and R. D. Madan, Selected Topics in Inorganic Chemistry, 8th Ed., S. Chand & Company ltd.
- 3. M. L. Tobe and J. Burgess, Inorganic Reaction Mechanism, Longman, 1999.
- 4. S. Asperger, Chemical kinetics and Inorganic Reaction Mechanism, 2nd Ed., Kluwer Academic/Plenum Publishers, 2002
- 5. F. Basalo and R. G. Pearson, Mechanism of Inorganic Reactions, 2nd Ed., Wiley, 1967.
- 6. R. Gopalan and V. Ramlingam, Concise Coordination chemistry, Vikas Publishing house Pvt Ltd., 2001.
- 7. Robert B. Jordan, Reaction Mechanisms of Inorganic and Organometallic Systems, 3rd Ed., Oxford University Press 2008.
- 8. D. Banerjea, Coordination chemistry. Tata McGrew Hill, New Delhi, 1993.
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- 10. R.H Crabtree, The Organometallic Chemistry of the Transition Metals, 5th edition, Wiley International Pvt, Ltd 2000.
- 11. B.Doughlas, D.H McDaniel and J.J Alexander. Concepts and Models of Inorganic Chemistry, 2nd edition, John Wiley and Sons. 1983.
- 12. Organometallic Chemistry by G.S Sodhi. Ane Books Pvt Ltd.
- 13. Environmental Chemistry 5th edition, Colin Baird Michael Cann, W. H. Freeman and Company, New York, 2012.
- 14. Environmental Chemistry 7th edition, Stanley E. Manahan, CRC Press Publishers,
- 15. Environmental Contaminants, Daniel A. Vallero, ISBN: 0-12-710057-1, Elsevier Inc., 2004.
- 16. Environmental Science 13th edition, G. Tyler Miller Jr. and Scott E. Spoolman, ISBN10: 0-495-56016-2, Brooks/Cole, Cengage Learning, 2010.
- 17. Fundamentals of Environmental and Toxicological Chemistry 4th edition, Stanley E. Manahan, ISBN: 978-1-4665-5317-0, CRC Press Taylor & Francis Group, 2013.
- 18. Living in the Environment 17th edition, G. Tyler Miller Jr. and Scott E. Spoolman, ISBN-10: 0-538-49414-X, Brooks/Cole, Cengage Learning, 2011
- 19. R. W. Hay, Bioinorganic Chemistry, Ellis Harwood, England, 1984.
- 20. I. Bertini, H.B.Gray, S. J. Lippard and J.S. Valentine, Bioinorganic Chemistry, First South Indian Edition, Viva Books, New Delhi, 1998.

- 21. J. A. Cowan, Inorganic Biochemistry-An introduction, VCH Publication, 1993.
- 22. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Publications, Mill Valley, Caligronic, 1994.
- 23. G.N. Mukherjee and A. Das, Elements of Bioinorganic Chemistry, Dhuri& Sons, Calcutta, 1988.
- 24. J.Chem. Educ. (Special issue), Nov, 1985.
- 25. E.Frienden, J.Chem. Educ., 1985, 62.
- 26. Robert R.Crechton, Biological Inorganic Chemistry An Introduction, Elsevier

NAME OF THE COURSE	INORGANIC CHEMISTRY PRACTICAL	
CLASS	MSC	
COURSE CODE	SMSCHEP202	
NUMBER OF CREDITS	2	
NUMBER OF LECTURES PER	4	
WEEK		
TOTAL NUMBER OF LECTURES	60	
PER SEMESTER		
EVALUATION METHOD	INTERNAL	SEMESTER END
	ASSESSMENT	EXAMINATION
TOTAL MARKS	-	50
PASSING MARKS		20

CO 1.	To train students to prepare and analyze inorganic complexes of various geometries
CO 2.	To use various optical methods for analysis of inorganic compounds

CLO 1.	Prepare and analyze inorganic complexes
CLO 2.	Perform analysis of various compounds using suitable optical method

INORGANIC CHEMISTRY PRACTICAL
(Any seven)
Il 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) ₄ CO ₃]NO3
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
- 2) Determination of K+ in fertilizer sample by standard addition method (flame photometer)
- 3) Simultaneous determination of Ni and Co by spectrophotometry
- 4)Kinetics of formation of Cr(III)-EDTA complex by spectrophotometry

REFERENCE:

- 1. Advanced experiments in Inorganic Chemistry., G. N. Mukherjee., 1 Edn., 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: <u>Dr Deepak Pant</u>

NAME OF THE COURSE	ORGANIC CHEMISTRY	
CLASS	MSC	
COURSE CODE	SMSCHE203	
NUMBER OF CREDITS	4	
NUMBER OF LECTURES PER	4	
WEEK		
TOTAL NUMBER OF LECTURES	60	
PER SEMESTER		
EVALUATION METHOD	INTERNAL	SEMESTER END
	ASSESSMENT	EXAMINATION
TOTAL MARKS	50	50
PASSING MARKS	20	20

COURSE OBJECTIVES:

CO 1.	Understanding the formation of enolate and the regioselectivity of alkylation of	
	enolates, Enamines, imines and their nitrogen analogs.	
CO 2.	Understand the mechanisms of reactions and the effect of various parameters on the	
	rate of the reaction, stereochemistry and selectivity of the product.	
CO 3.	Understanding chemical reactions with the help of FMOand HUMO - LUMO gap in	
	UV absorption spectra and interpreting the reactivity of the given compounds.	
CO 4.	Understand the basic concepts of Molecular spectroscopy.	

CLO 1.	Predict the formation of enolates, mechanism, rate of the reaction, stereochemical	
	outcome of reactions and write the Industrial application of reactions	
CLO 2.	Able to draw the FMO's of alkenes, Formaldehyde, allyl anion and cation and apply	
	the concept of FMO's to substitution and addition reactions.	
CLO 3.	Analyse the effect certain factors on spectrum of the compound	
CLO 4.	Interpretation of spectral data and elucidation of structure	

UNIT	ALKYLATION AND REACTIONS OF CARBON NUCLEOPHILES	15L
1		
1.1	Alkylation of Nucleophilic Carbon Intermediates:	7 L
1.1.1.	Generation of carbanion, kinetic and thermodynamic enolate formation, Regioselectivity in enolate formation, alkylation of enolates.	
1.1.2	Generation and alkylation of dianion, medium effects in the alkylation of enolates, oxygen versus carbon as the site of alkylation.	
1.1.3	Alkylation of aldehydes, ketones, esters, amides and nitriles.	
1.1.4	Nitrogen analogs of enols and enolates- Enamines and Imines anions, alkylation of enamines and imines.	
1.1.5	Alkylation of carbon nucleophiles by conjugate addition (Michael reaction).	
1.2	Reaction of carbon nucleophiles with carbonyl groups:	8 L
1.2.1	Mechanism of Acid and base catalyzed Aldol condensation, Mixed Aldol condensation with aromatic aldehydes, regiochemistry in mixed reactions of aliphatic aldehydes and ketones, intramolecular Aldol reaction and Robinson annulation.	
1.2.2	Addition reactions with amines and iminium ions; Mannich reaction.	
1.2.3	Amine catalyzed condensation reaction: Knoevenagel reaction.	
1.2.4	Acylation of carbanions.	
UNIT 2	REACTIONS AND REARRANGEMENTS	15L
	Mechanisms, stereochemistry (if applicable) and applications of the following:	9L
2.1	Reactions: Baylis-Hilman reaction, McMurry Coupling, Corey-Fuchs reaction, Nef reaction, Passerini reaction.	
2.2	Concerted rearrangements: Hofmann, Curtius, Lossen, Schmidt, Wolff, BoultonKatritzky	
2.3	Cationic rearrangements: Tiffeneau-Demjanov, Pummerer, Dienone-phenol, Rupe, Wagner-Meerwein.	
2.4	Anionic rearrangements: Brook, Neber, Von Richter, Wittig, Gabriel-Colman, Payne. [Reference Books: 19-22]	
UNIT 3	MOLECULAR ORBITAL THEORY AND UV IR SPECTROSCOPY	15L

3.1	Introduction to Molecular Orbital Theory for Organic Chemistry	7L
3.1.1	Molecular orbitals: Formation of σ - and π -MOs by using LCAO method. Formation of π MOs of ethylene, butadiene, 1, 3, 5-hexatriene, allyl cation, anion and radical. Concept of nodal planes and energies of π -MOs	
3.1.2	Introduction to FMOs: HOMO and LUMO and significance of HOMO-LUMO gap in absorption spectra as well as chemical reactions. MOs of formaldehyde: The effect of electronegativity perturbation and orbital polarization in formaldehyde. HOMO and LUMO (π and π^* orbitals) of formaldehyde. A brief description of MOs of nucleophiles and electrophiles. Concept of 'donor-acceptor' interactions in nucleophilic addition reactions on formaldehyde. Connection of this HOMO-LUMO interaction with 'curved arrows' used in reaction mechanisms. The concept of hardness and softness and its application to electrophiles and nucleophiles. Examples of hard and soft nucleophiles/ electrophiles. Identification of hard and soft reactive sites on the basis of MOs.	
3.3	Application of FMO concepts in (a) S_N^2 reaction, (b) Lewis acid base adducts (BF ₃ NH ₃ complex), (c) ethylene dimerization to butadiene, (d) Diels-Alder cycloaddition, (e) regioselective reaction of allylcation with allyl anion (f) addition of hydride to formaldehyde.	
3.2	Applications of UV and IR spectroscopy:	8 L
3.2.1	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).	
3.2.2	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.	
UNIT	NMR SPECTROSCOPY AND MASS SPECTROMETRY	15L
4	B 1 Cl 1 1:0	
4.1	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.	
4.2	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.	
4.3	Mass spectrometry: Molecular ion peak, base peak, isotopic abundance, metastable ions. Nitrogen rule, 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, ortho effect.	
4.4	Structure determination involving individual or combined use of the above spectral techniques. [Reference Books: 13-18]	

REFERNCES (LIMIT TO 10)

- 1. Organic Chemistry, J. Claydens, N. Greeves, S. Warren and P. Wothers, Oxford University Press.
- 2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Part A, page no. 713-769, and B, Plenum Press.
- 3. March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, Michael B. Smith, Jerry March, Wiley.
- 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.
- 10. Advanced Organic Chemistry: Reactions and mechanism, L.G. Wade, Jr., Maya Shankar Singh, Pearson Education.
- 11. Mechanism in Organic Chemistry, Peter Sykes, 6th
- 12. Molecular Orbital and Organic chemical reactions, Ian Fleming Reference Edition, Wiley
- 13. Introduction to Spectroscopy, Donald L. Pavia, Gary M. Lampman, George S. Kriz, Thomson Brooks.
- 14. Spectrometric Identification of Organic Compounds, R. Silverstein, G.C Bassler and T.C. Morrill, John Wiley and Sons.
- 15. Organic Spectroscopy, William Kemp, W.H. Freeman & Company.
- 16. Organic Spectroscopy-Principles and Applications, Jagmohan, Narosa Publication.
- 17. Organic Spectroscopy, V.R. Dani, Tata McGraw Hill Publishing Co.
- 18. Spectroscopy of Organic Compounds, P.S. Kalsi, New Age International Ltd.
- 19. Organic Reaction Mechanisms, V.K. Ahluwalia, R.K. Parasher, Alpha Science

International, 2011.

- 20. Reactions, Rearrangements and Reagents by S. N. Sanyal
- 21. Name Reactions, Jie Jack Li, Springer
- 22. Name Reactions and Reagents in Organic Synthesis, Bradford P. Mundy, M.G. Ellerd, and F.G. Favaloro, John Wiley & Sons.

NAME OF THE COURSE	ORGANIC CHEMISTRY PRACTICAL	
CLASS	MSC	
COURSE CODE	SMSCHEP203	
NUMBER OF CREDITS	2	
NUMBER OF LECTURES PER	4	
WEEK		
TOTAL NUMBER OF LECTURES	60	
PER SEMESTER		
EVALUATION METHOD	INTERNAL	SEMESTER END
	ASSESSMENT	EXAMINATION
TOTAL MARKS	-	50
PASSING MARKS		20

COURSE OBJECTIVES:

Learners will learn to:

CO 1.	Understand the method and concept of separation and learn to separate a binary mixture quantitatively by chemical method.
CO 2.	Learn to perform qualitative analysis, prepare a derivative and identify one of the components
CO 3.	Learn the method of purification of the components.
CO 4.	Learn to interpret the spectrum.

CLO 1.	To identify the nature of a binary mixture and separate the mixture quantitatively.
CLO 2.	To perform organic qualitative analysis
CLO 3.	To purify compounds by distilling/recrystallization techniques.
CLO 4	To elucidate the structure of a compound based on spectra

ORGANIC CHEMISTRY PRACTICAL	
Separation of Binary mixture using micro-scale technique	
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:
 - (i) Water soluble/water insoluble solid and water insoluble solid, (ii) Non-volatile liquid-Non-volatile liquid (chemical separation) (iii) Water-insoluble solid-Non-volatile liquid.

Minimum three mixtures from each type and a total of ten mixtures are expected.

REFERNCE:

- 1. Systematic Qualitative organic analysis, H. Middleton (Orient Longman)
- 2. A Handbook of Organic Analysis, H.T. Clark (Orient Longman)
- 3. Systematic Identification of organic compounds, R.L. Shriner (John Wiley, New York)
- 4. Practical Organic Chemistry by Mann and Saunders.
- 5. Advance Practical Organic Chemistry, N.K. Vishnoi, Vikas Publication

NAME OF THE COURSE	ANALYTICAL CHEM	ISTRY
CLASS	MSC	
COURSE CODE	SMSCHE204	
NUMBER OF CREDITS	4	
NUMBER OF LECTURES PER	4	
WEEK		
TOTAL NUMBER OF LECTURES	60	
PER SEMESTER		
EVALUATION METHOD	INTERNAL	SEMESTER END
	ASSESSMENT	EXAMINATION
TOTAL MARKS	50	50
PASSING MARKS	20	20

COURSE OBJECTIVES:

CO 1.	To learn the principle and working of various chromatographic methods for separation	
	and identification of mixture of unknown compounds by using suitable detectors.	
CO 2.	To understand application of different X-ray spectroscopic methods as a tool for	
	surface studies.	

CO 3.	To learn the principle and working of MSwith different analysers as a tool for
	structural elucidation of organic compounds.
CO 4.	To learn about advanced electroanalytical methods to analyse mixtures.

COURSE LEARNING OUTCOMES:

The learner will be able to

CLO 1.	explain various chromatographic, ICP-AES and X-ray spectroscopic methods with
	emphasis on principle and working of the instrument.
	carry out structural elucidation of simple organic compounds from the MS data.
CLO2.	Draw a simple block/schematic diagram of the instruments learnt and explain the
	importance of each component.
CLO 3.	Comprehend applications of isotope dilution method and solve numerical problems for
	a given data.
CLO4	Explain various types of electroanalytical methods and compare advantages and
	limitations of one over the other.

UNIT 1	CHROMATOGRAPHY	15L
1.1	Recapitulation of basic concepts in chromatography: Classification of chromatographic methods, requirements of an ideal detector, types of detectors in LC and GC, comparative account of detectors with reference to their applications (LC and GC respectively), qualitative and quantitative analysis.	2L
1.2	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.	5L
1.3	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.	3L
1.4 4	High Performance Liquid Chromatography (HPLC): Normal phase and reversed phase with special reference to types of commercially available columns (Use of C8 and C18 columns). Diode array type and fluorescence detector, Applications of HPLC. Chiral and ion chromatography.	5L
UNIT 2	SPECTROMETRY AND RADIO-ANALYTICAL METHODS	15L
2.1	X-ray spectroscopy : principle, instrumentation and applications of X-ray fluorescence, absorption and diffraction spectroscopy.	4L
2.2	Mass spectrometry: recapitulation, instrumentation, ion sources for molecular studies, electron impact, field ionization, field absorption, chemical ionization and fast atom bombardment sources. Mass analyzers: Quadrupole, time of flight and ion trap. Applications.[6L

2.3	Radioanalytical Methods – recapitulation, isotope dilution method, introduction, principle, single dilution method, double dilution method and applications.	5L
UNIT 3	SURFACE ANALYTICAL TECHNIQUES	15L
3.1	Surface Analytical Techniques – [9 L]	3L
	Introduction, Principle, Instrumentation and Applications of:	
3.1.1	Scanning Electron Microscopy (SEM)	
3.1.2	Scanning Tunneling Microscopy (STM)	
3.1.3	Transmission Electron Microscopy (TEM)	
3.1.4	Electron Spectroscopy (ESCA and Auger)	
3.2	Atomic Spectroscopy	6L
3.2.1	Advantages and Limitations of AAS	
3.2.2	Atomic Spectroscopy based on plasma sources - Introduction, Principle,	
	Instrumentation and Applications.	
	ELECTROANALYTICAL METHODS	
4.1	Ion selective potentiometry and Polarography	10 L
	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.	
	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, applications.	3L
4.3	Coulometry: Introduction, principle, instrumentation, coulometry at controlled potential and controlled current	21

REFERNCES

- 1. Instrumental Analysis, Skoog, Holler & Drouch
- 2. HPLC Practical and Industrial Applications, 2 nd Ed., Joel K. Swadesh, CRC Press
- 3. Essentials of Nuclear Chemistry, H J Arnikar, New Age Publishers (2005)
- 4. Fundamentals of Radiochemistry D. D. Sood , A. V. R. Reddy and N. Ramamoorthy
- 5. Principles of Instrumental Analysis Skoog, Holler and Nieman, 5th Edition, Ch: 12
- 6. Principles of Instrumental Analysis Skoog, Holler and Nieman, 5th Edition, Ch: 20
- 7. Instrumental Analysis by Douglas A. Skoog F. James Holler Crouch, Publisher: Cengage; Edition, (2003), ISBN-10: 8131505421, ISBN-13: 978-8131505427
- 8. Physical Principles of Electron Microscopy, An Introduction to TEM, SEM, and AEM
- 9. Authors: Ray F. Egerton, ISBN: 978-0-387-25800-3 (Print) 978-0-387-26016-7 (Online)

- 10. Modern techniques of surface science by D.P. Woodruff, T.A. Delchar, Cambridge Univ. Press, 1994.
- 11. Introduction to Scanning Tunneling Microscopy by C. J. Chen, Oxford University Press, NewYork, 1993.
- 12. Transmission Electron Microscopy: A text book for Material Science, David B Williams and C., Barry Carter, Springer
- 13. Modern Spectroscopy, by J.M. Hollas, 3rd Edition (1996), John Wiley, New York
- 14. Principles of Instrumental Analysis Skoog, Holler, Nieman, 5th ed., Harcourt College Publishers, 1998.
- 15. Instrumental Analysis by Douglas A. Skoog F. James Holler Crouch, Publisher: Cengage; Edition (2003), ISBN10: 8131505421, ISBN-13: 978-8131505427
- 16. Principles of Instrumental Analysis Skoog, Holler, Nieman, 5th Edition, Harcourt College Publishers, 1998. Chapters 23, 24, 25.
- 17. Analytical Chemistry Principles John H Kennnedy, 2nd edition, Saunders College Publishing (1990).
- 18. Modern Analytical Chemistry David Harvey; McGraw Hill Higher education publishers, (2000).
- 19. Vogel's Text book of quantitative chemical analysis, 6th edition, Pearson Education Limited, (2007).
- 20. Electrochemical Methods Fundamentals and Applications, Allen J Bard and Larry R Faulkner, John Wiley and Sons, (1980).
- 21. Instrumental Methods of Analysis Willard, Merrit, Dean and Settle, 7th edition, CBS publishers.

NAME OF THE COURSE	ANALYTICAL CHEM	ISTRY PRACTICAL
CLASS	MSC	
COURSE CODE	SMSCHEP204	
NUMBER OF CREDITS	2	
NUMBER OF LECTURES PER	4	
WEEK		
TOTAL NUMBER OF LECTURES	60	
PER SEMESTER		
EVALUATION METHOD	INTERNAL	SEMESTER END
	ASSESSMENT	EXAMINATION
TOTAL MARKS	-	50
PASSING MARKS		20

CO 1.	To learn analysis of the mixture of two or more species using a classical or
	instrumental method.
CO 2.	To learn handling of different instruments.
CO 3.	To use a given method to comment on the quality of the compound.

COURSE LEARNING OUTCOMES:

The learner will be able to

CLO 1.	Analyse a given mixture with the highest degree of accuracy by using classical or
	instrumental method of analysis.
CLO 2.	Check the quality of any given compound.
CLO 3.	Handle various instruments confidently.
CLO 4.	Perform analysis at various concentrations.

	ANALYTICAL CHEMISTRY PRACTICAL
	1. To determine percentage purity of sodium carbonate in washing soda pH metrically.
	2. To determine amount of Ti(III) and Fe(II) in a mixture by titration with Ce(IV) potentiometrically.
	3. To determine the percentage purity of a sample (glycine/sodium benzoate/primary amine) by titration with perchloric acid in a non aqueous medium using glass calomel system potentiometrically.
	4. To determine the amount of nitrite present in the given water sample colorimetrically.
	5. To determine the amount of Fe(II) and Fe(III) in a mixture using 1,10-phenanthroline spectrophotometrically.
	6. Simultaneous determination of Cr(VI) and Mn(VII) in a mixture spectrophotometrically.
	7. To determine the percentage composition of HCl and H ₂ SO ₄ on weight basis in a mixture of two by conductometric titration with NaOH and BaCl ₂ .
	8. To determine amount of potassium in the given sample of fertilizers using flame photometer by standard addition method.
1	

REFERENCES:

- 1. Quantitative Inorganic Analysis including Elementary Instrumental Analysis by A. I. Vogels, 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

ASSESSMENT DETAILS:(this will be same for all the theory papers)

Internal Assessment (50 marks)

Part 1: Project Work (50 Marks)

• At the beginning of the semester, students should be assigned project topics

drawn from Unit 1 to Unit 4.

- Students work individually.
- Project Marks will be divided as written submission:15 Marks; Presentation, content
 & Viva: 15 marks; 10 Marks for active participation)
- 2. Two tests of 10 Marks was conducted and average of the marks was considered

Semester End Examination – External Assessment (50 marks)

Semester I

Online Examination

Pattern: MCQ for 30 marks

The test paper will consist of 1 and 2 mark questions equal distribution from all units

Subjective type for 20 marks.

One 5M question from each of the 4 units

Semester II

Online Examination

Pattern: MCQ for 50 marks

The test paper will consist of 1 and 2 mark questions equal distribution from all units

Practical Assessment (for papers with practicals)

Practical examination of each paper for 50 marks

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