

**Programme Code: SMSCHE** 

M.Sc. Part I

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

# **Programme Outline:** MSc (SEMESTER I)

Course Code	Unit No	Name of the Unit	Credit
			S
SMSCHE101		PHYSICAL CHEMISTRY	4
	1	Thermodynamics – I	
	2	Quantum Chemistry – I	
	3	Chemical Dynamics – I	
	4	Electrochemistry	
SMSCHE102		INORGANIC CHEMISTRY	4
	1	Chemical Bonding	
	2	Molecular Symmetry and Group Theory	
	3	Materials Chemistry and Nanomaterials	
	4	Characterisation of Coordination Compounds	
SMSCHE103		ORGANIC CHEMISTRY	4
	1	Physical Organic Chemistry	
	2	Nucleophilic Substitution Reactions and	
		Aromaticity	
	3	Stereochemistry	
	4	Oxidation and Reduction	
SMSCHE104		ANALYTICAL CHEMISTRY	4
	1	Language and Quality in Analytical	
		Chemistry	
	2	Calculations based on Chemical Principles	
	3	Optical methods	
	4	Thermal methods	
SMSCHEP101		PHYSICAL CHEMISTRY PRACTICAL	2
SMSCHEP102		INORGANIC CHEMISTRY PRACTICAL	2
SMSCHEP103		ORGANIC CHEMISTRY PRACTICAL	2
SMSCHEP104		ANALYTICAL CHEMISTRY PRACTICAL	2

# **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	1
	4	Bioinorganic Chemistry	1
SMSCHE203		ORGANIC CHEMISTRY	4
	1	Alkylation and reaction of carbon nucleophiles	
	2	Reactions and Rearrangements	
	3	Molecular Orbital Theory	
	4	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	<b>Skills in research and industrial field:</b> 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	<b>Personality Development:</b> The students will be able to handle personal, social, environmental issues and will be responsible citizens.	

#### **SEMESTER 1**

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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

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 I	THERMODYNAMICS – I	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.	
	Third law of Thermodynamics, Entropy change for a phase transition, absolute	
	entropies, determination of absolute entropies in terms of heat capacity, standard	
1.2		
	molar entropies and their dependence on molecular mass and molecular structure,	
	residual entropy.	
	Entropies of vaporization of liquids – Trouton's rule, Validity, deviation and	
1.3	application, Hildebrand's rule	
	[Ref 2 and 1,10,11,12 17]	
UNIT		
II	QUANTUM CHEMISTRY	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	
2.2	functions, Normalization of wave functions, orthogonality of wave functions.	
	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, Eigenvalues and Eigen value equation, Schrödinger wave	
2.3	equation as the Eigenvalue 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.	
	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	
2.4	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
III		132
	Composite Reactions:	
	Steady state Approximation, rate determining steps, Microscopic Reversibility and	
	Detailed Balanced Chain reactions-chain initiation processes. Some inorganic	
3.1	mechanisms: formation and decomposition of phosgene, decomposition of ozone,	
3.1	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.	
,		
	Polymerization reactions:	
3.2	<b>Polymerization reactions:</b> 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.	
	Reaction in Gas Phase:	
	Unimolecular Reactions: Lindeman-Hinshelwood theory, Rice-Ramsperger-Kasssel	
3.3	(RRK) theory, Rice-Ramsperger-Kassel Marcus (RRKM) theory.	
	[Ref. 2 and 15, 17, 18]	
UNIT	ELECTROCHEMISTRY	15L
IV	ELECTROCHEMISTRI	ISL
4.1	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: 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.	
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.)	
	REFERENCES	

- 1. Peter Atkins and Julio de Paula, Atkin's Physical Chemistry, 7<sup>th</sup> Edition, 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<sup>rd</sup> Edition, John Wiley and Sons (Asia) Pte. Ltd., 2002.
- 4. Ira R. Levine, Physical Chemistry, 5th Edition, Tata McGraw-Hill New Delhi, 2002.
- 5. G.W. Castellan, Physical Chemistry, 3<sup>rd</sup> Edition, Narosa Publishing House, New Delhi, 1983.
- 6. S. Glasstone, Textbook of Physical Chemistry, 2ndEdition., 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, 2<sup>nd</sup> Edition, 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<sup>th</sup> Edition, Pearson Education (Singapore) Pte. Ltd., Indian Branch, New Delhi, 2000.
- 14. Thomas Engel and Philip Reid, Physical Chemistry, 3<sup>rd</sup> Edition, Pearson Education Limited 2013.
- 15. D.N. Bajpai, Advanced Physical Chemistry, S. Chand 1st Edition, 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 Textbook of Physical Chemistry by K L kapoorVol 5, 2ndEdition

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
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:
1.	Determine the heat of solution ( $\Delta H$ ) of a sparingly soluble acid (benzoic /salicylic acid) from solubility measurement at three different temperatures.
2.	Investigate the reaction between acetone and iodine.
	Study the variation in the solubility of Ca(OH) <sub>2</sub> in presence of NaOH and hence to determine the solubility product of Ca(OH) <sub>2</sub> at room temperature.
4.	Determine the partial molal volume of Ethanol - water mixture at a given composition.
Instru	mental:
1.	Determine the mean ionic activity coefficient of an electrolyte by e.m.f. measurement.
2.	Determine pKa values of phosphoric acid by potentiometric titration with sodium hydroxide using glass electrodes.
3.	Verify Ostwald's dilution law and to determine the dissociation constant of a weak mono-basic acid conductometrically.
4.	Determine the stability constant of the complex formed between Fe <sup>3+</sup> ion and 5-sulphosalicylic acid at pH 2 and pH 3 by spectrophotometric method

### **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, 3<sup>rd</sup>Edn., Longman Group Ltd., 1974.
- 3. Experimental Physical Chemistry, V.D. Athawale and P. Mathur, New Age

# International Publishers, 2001.

NAME OF THE COURSE	INORGANIC 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 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 1	CHEMICAL BONDING	
1.1	<b>Valence Bond Theory</b> Recapitulation of hybridization, Derivation of wave functions for $sp$ , $sp^2$ , $sp3$ orbital hybridization types considering only sigma bonding, and Critical analysis of VBT.	4L
1.2	Bent's rule:	3L

		I	
	Structure and reactivity of compounds/ complexes		
	Molecular Orbital Theory:		
	Molecular Orbital Theory (considering σ bonding) for		
1.3	- diatomic species of the first transition series	5I	
	-polyatomic species: electron deficient (B <sub>2</sub> H <sub>6</sub> ) and electron rich (I <sub>3</sub> ) molecular		
	species.		
	Weak forces of attraction:		
	i) Hydrogen bonding – concept, types, properties, methods of detection and		
1.4	importance.	31	
	ii) Van der Waal's forces, ion-dipole, dipole-dipole and London forces.		
UNIT 2	MOLECULAR SYMMETRY AND GROUP THEORY	15	
	Symmetry criterion of optical activity, symmetry restrictions on dipole		
2.1	moment, elements of symmetry, A systematic procedure for symmetry	31	
	classification of molecules.		
	Concepts of Groups, Sub-groups, Classes of Symmetry operations,		
2.2	Group Multiplication Tables. Abelian and non-Abelian point groups.	31	
	Representation of Groups: Matrix representation of symmetry operations,		
	reducible and irreducible representations. The Great Orthogonality Theorem		
2.3	and its application in construction of character tables for point groups $C_2v$ ,	51	
	$C_3$ v and $D_{2h}$ , structure of character tables.		
	Applications of Group Theory		
	(a) Symmetry adapted linear combinations (SALC), symmetry aspects of		
	MOT, sigma bonding in AB <sub>n</sub> (Ammonia, CH <sub>4</sub> ) molecule.		
	(b) Determination of symmetry species for translations and rotations.		
2.4	(c) Mulliken's notations for irreducible representations.	4]	
	(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	15	
3.1	Solid State Chemistry	10	
3.1.1	Electronic structure of solids and band theory, Fermi level, K Space and		
3.1.2	Brillouin Zones.		
	Structures of Compounds of the type: AB [nickel arsenide (NiAs)], AB <sub>2</sub>		
	[fluorite (CaF <sub>2</sub> ) and anti-fluorite structures, rutile (TiO <sub>2</sub> ) structure and layer		
3.1.3	structure [cadmium chloride and iodide (CdCl <sub>2</sub> , CdI <sub>2</sub> )].		
	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)	<b></b>	
2.2	Nanaga Assis Isa		
3.2.1	Nanomaterials:  Methods of preparation of nanomaterials: Chemical methods, Solvothermal,	5I	

	Combustion synthesis, Microwave, Co-precipitation, Langmuir Blodgett (L-			
	B) method, Biological methods: Synthesis using microorganisms. SEM,			
	TEM			
UNIT 4	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.	4L		
	Spectral calculations using Orgel and Tanabe-Sugano diagram,			
4.2	calculation of electronic parameters such as $\Delta$ , B, C, Nephelauxetic ratio.			
4.3	Magnetic Properties of Coordination Complexes: Origin of magnetism, types of magnetism, Curie law, Curie-Weiss Law, 1stand 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.	<b>6</b> L		
	REFERENCES			
UNIT I	<ol> <li>B. R. Puri, L. R. Sharma and K. C. Kalia, Principles of Inorganic Che Milestone Publishers, 2013-2014.</li> <li>B. W. Pfennig, Principles of Inorganic Chemistry, Wiley, 2015.</li> <li>C. E. Housecroft and A. G. Sharpe, Inorganic Chemistry, Pearson Edu Limited, 2nd Edition 2005.</li> <li>J. Huheey, F. A. Keiter and R. I. Keiter, Inorganic Chemistry-Princi Structure and Reactivity, 4th Ed., Harper Collins, 1993.</li> <li>P. J. Durrant and B. Durrant, Introduction to Advanced Inorganic Che Oxford University Press, 1967.</li> <li>R. L. Dekock and H.B.Gray, Chemical Structure and Bonding, The Be Cummings Publishing Company, 1989.</li> <li>G. Miessler and D. Tarr, Inorganic Chemistry, 3rd Ed., Pearson Edu 2004.</li> <li>R. Sarkar, General and Inorganic Chemistry, Books &amp; Allied (P) Ltd., 2</li> </ol>	ples of mistry, enjamin ecation, 2001.		
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	Publishing House. 2014.			
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	0-20349635-3, Taylor & Francis Group, LLC.			
	2. Nanomaterials &Nanochemistry, 2007, Catherine Brechignac, Philippe			
	Houdy, Marcel Lahmani, ISBN 978-3-540-72992-1 Springer Berlin			
	Heidelberg New York.			
	3. Nanomaterials Chemistry, Recent Developments and New Directions C.N.R.			
UNIT III	Rao, A. Muller, and A.K. Cheetham, ISBN 978-3-527-31664-9, 2007			
UNITIII	WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.			
	4. Nano-Surface Chemistry, 2001, Morton Rosoff, ISBN: 0-8247-0254-9,			
	Marcel Dekker Inc. New York.			
	5. The Chemistry of Nanomaterials, CNR Rao, Muller Cheetham, WILEY-VCH			
	Verlag GmbH & Co. KGaA, Weinheim, 2004.			
	6. Semiconductor Nanomaterials, Challa S.S.R. Kumar, ISBN: 978-3-527-			
	32166-7, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2010.			
	1. J. E. Huheey, E. A. Keiter and R. L. Keiter; Inorganic Chemistry: Principles			
	of Structure and Reactivity, Pearson Education, 2006.			
	2. D. Banerjea ,Coordination Chemistry			
	3. Geary Coordination reviews			
	4. P.W. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong; Shriver &			
UNITIV	Atkins: Inorganic Chemistry, 4th ed. Oxford University Press, 2006.			
	5. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann; Advanced			
	Inorganic Chemistry, 6th ed. Wiley, 1999,			
	6. B. Douglas, D. McDaniel and J. Alexander. Concepts and Models of			
	Inorganic Chemistry (3rd Edition.), John Wiley & Sons (1994).			
UNIT IV	<ol> <li>Geary Coordination reviews</li> <li>P.W. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong; Shriver &amp; Atkins: Inorganic Chemistry, 4th ed. Oxford University Press, 2006.</li> <li>F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann; Advanced Inorganic Chemistry, 6th ed. Wiley, 1999,</li> <li>B. Douglas, D. McDaniel and J. Alexander. Concepts and Models of</li> </ol>			

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
(Any seven)
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.
6) Synthesis of Fe2O3 nanoparticles by sol-gel/ coprecipitation/ hydrothermal method (any one)
7) Synthesis of ZnO from zinc oxalate - precursor method and determine band gap by absorption spectroscopy
II] Instrumentation:
1) Estimation of Copper using Iodometric method Potentiometrically.
2) Estimation of boric acid conductometrically.

### **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	<b>EXAMINATION</b>
TOTAL MARKS	50	50
PASSING MARKS	20	20

CO 1.	Understand the mechanisms of reactions and the effect of various parameters on the
	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 symmetric
	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

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	

	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 structures	
	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.	6L
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.	3L
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.	
UNIT 2	NUCLEOPHILIC SUBSTITUTION REACTIONS AND AROMATICITY	
2.1	Nucleophilic substitution reactions	
2.1.1 2.1.2 2.1.3	Aliphatic nucleophilic substitution: S <sub>N</sub> 1, S <sub>N</sub> 2, (including effects of solvents on these reactions Factors affecting these reactions: substrate, nucleophilicity, solvent, steric effect, leaving group and hard-soft interaction.) S <sub>N</sub> <sup>i</sup> reactions, mixed S <sub>N</sub> 1 and S <sub>N</sub> 2 and SET mechanisms. S <sub>N</sub> reactions involving NGP - participation by aryl rings, αand pi-cyclopropene bonds. Ambident nucleophiles. S <sub>N</sub> CA, S <sub>N</sub> at sp <sup>2</sup> (vinylic) carbon.  Aromatic nucleophilic substitution: S <sub>N</sub> Ar, S <sub>N</sub> 1, benzyne mechanisms. Ipso, cine.  Ester hydrolysis: Classification, nomenclature and study of all eight mechanisms of acid and base catalyzed hydrolysis with suitable examples.	
2.2	Aromaticity:	5L
2.2.1	Structural, thermochemical, and magnetic criteria for aromaticity, including NMR characteristics of aromatic systems. Delocalization and aromaticity.	2L
	Application of HMO theory to monocyclic conjugated systems. Frost-Musulin	

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 ( $C_{60}$ ).	2L	
	[Reference Books 1,2,13,16]		
UNIT 3	STEREOCHEMISTRY		
3.1	Molecules with tri- and tetra-coordinate centers: Compounds with carbon, silicon, nitrogen, phosphorus and sulphur chiral centers, relative configurational stabilities.		
3.2	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 pseudo asymmetric centres.		
3.3	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.		
3.4	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.  [Reference Books: 6-8]		
IINIT 4		151	
UNIT 4	OXIDATION AND REDUCTION	15L	
4.1	Oxidation	8L	
4.1.1	<b>Oxidation:</b> General mechanism and selectivity of hydrocarbons, alcohols, carbonyl compounds		
4.1.2	Oxidation of hydrocarbons:  Dehydrogenation: Dehydrogenation of C-C bonds including aromatization of six  mark and single variety metal (Pt. Pd. Ni) and argenia respects (chlargeil, DDO)		
4.1.3	membered rings using metal (Pt, Pd, Ni) and organic reagents (chloranil, DDQ).  Oxidation involving C-C bonds cleavage: Glycols using HIO <sub>4</sub> ; cycloalkanones using CrO <sub>3</sub> ; carbon-carbon double bond using ozone, KMnO <sub>4</sub> , NaIO <sub>4</sub> and OsO <sub>4</sub> ;		
4.1.4	aromatic rings using RuO <sub>4</sub> and NaIO <sub>4</sub> . <b>Oxidation involving replacement of hydrogen by oxygen:</b> oxidation of CH <sub>2</sub> to CO by SeO <sub>2</sub> , oxidation of aryl methanes by CrO <sub>2</sub> Cl <sub>2</sub> (Etard oxidation).		
4.1.5	Oxidation of alcohols: Chromium reagents such as $K_2Cr_2O_7/H_2SO_4$ (Jones		

	reagent), CrO <sub>3</sub> -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.	
4.1.6	Oxidation of aldehydes and ketones: with $H_2O_2$ (Dakin reaction), with peroxy	
	acid (Baeyer-Villiger oxidation)	
4.2	Reduction	
4.2.1	Reduction: General mechanism, selectivity, and important applications of the	
	following reducing reagents:	
4.2.2	Catalytic reduction: Clemmensen reduction, Adams Catalyst, Raney Nickel	
4.2.3	Reduction by hydride: Transfer reagents Boron reagents (NaBH <sub>4</sub> , NaCNBH <sub>3</sub> ,	
	diborane, 9-BBN, Na(OAc) <sub>3</sub> BH, aluminium reagents (LiAlH <sub>4</sub> , DIBAL-H, Red Al, L	
	and K- selectrides).	
4.2.4	<b>Dissolving metal reductions:</b> using Zn, Li, Na, and Mg under neutral and acidic	
	conditions, Li/Na-liquid NH <sub>3</sub> mediated reduction (Birch reduction) of aromatic	
	compounds and acetylenes.	
4.2.5	Other Methods of reduction: Wolff Kishner reduction and Huang-Minlon	
	modification. NH <sub>2</sub> NH <sub>2</sub> (diimide reduction) and other non-metal based agents	
	including organic reducing agents (Hantzsch Dihydropyridine).	

#### REFERENCES

- 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.

# PRACTICALS Course Code: SMSCHEP103

### **Learning Objectives:**

#### Learner will learn

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

#### **Learning Outcomes:**

#### Learner will be able to

- Prepare organic compounds at micro scale
- To assess the purity of the prepared compound
- Monitor the progress of the reaction using TLC

### I. 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-diphenylquinoxaline
- 10. Urea and benzil to 5,5-diphenylhydantoin
- II. Laboratory preparation of shaving gel
- III. Plotting TLC for organic synthesis

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	<b>EXAMINATION</b>
TOTAL MARKS	50	50
PASSING MARKS	20	20

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 I	LANGUAGE AND QUALITY OF/IN ANALYTICAL CHEMISTRY	15L
1.1	Language of Analytical Chemistry:	8L
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,	
1.1.3	transducers and sensors, selection of an analytical method, accuracy, precision, selectivity, sensitivity, detection limit and dynamic range.  Errors, determinate and indeterminate errors. Types of determinate errors,	

3.2.1	Beer- Lambert's Law, factors affecting molecular absorption, types of transitions	
3.2	Molecular Ultraviolet and Visible Spectroscopy: (Numericals are expected)	6 L
3.1.3	Introduction of Fourier Transform	
3.1.2	Laser as a source of radiation, Fibre optics	
	sample containers.	
3.1.1	Recapitulation of basic concepts, Electromagnetic spectrum, Sources, Detectors,	
3.1	Recapitulation and FT Technique:	3L
III	OPTICAL METHODS	15L
UNIT		
	solution of a oxidizing / reducing agent and its relationship with molarity).	
	of oxidation number, oxidizing and reducing agents, equivalent weight of oxidizing and reducing agents, stoichiometry of redox titration (Normality of a	
2.7	Oxidation number, rules for assigning oxidation number, redox reaction in term	
2 -	formation constants.	
2.6	Concept of formation constants, stability and instability constants, stepwise	1011
2.5	Calculations of pH of acids, bases, acidic and basic buffers.	15L
2.4	Solubility and solubility equilibria, effect of presence of common ion.	
	theoretical and practical yield.	
2.3	Stoichiometry of chemical reactions, concept of kg mol, limiting reactant,	
2.2	Calculations of ppm, ppb and dilution of the solutions, concept of mmol.	
2.1	Concentration of a solution based on volume and mass units.	
UNIT II	(The topics are to be covered in the form of numerical problems only.)	15L
	CALCULATIONS BASED ON CHEMICAL PRINCIPLES	
	Principle, Objective, OECD guidelines, The US FDA 21CFR58, Klimisch score	
1.2.4	Good Laboratory Practices (GLP):	
	Standards (ISI, Hallmark, Agmark)	
	Accreditation of Laboratories, Introduction to ISO series, Indian Government	
1.2.3	Accreditations:	
	(including process calorimetry / thermal build up concepts).	
	OSHA, Toxic Hazard (TH) classifications, Hazardous Chemical Processes	
	Basic concepts of Safety in Laboratories, Personal Protection Equipment (PPE),	
1.2.2	Safety in Laboratories:	
	reviews, responsibility of laboratory staff for quality and problems.	
	TQM (reference of Kaizen, Six Sigma approach & 5S), quality audits and quality	
	laboratories, total quality management (TQM), philosophy implementation of	
1.2.1	Quality Management System (QMS):  Evolution and significance of Quality Management, types of quality standards for	
1.2	Quality in Analytical Chemistry:	7 L
1.2	internal standard method.	<b>7</b> T
1.1.4	Quantitative methods of analysis: calibration curve, standard addition and	
4 4 4	tackling of errors	

	[emphasis on charge transfer absorption], pH, temperature, solvent and effect of		
	substituents.		
	Applications of Ultraviolet and Visible spectroscopy:		
	On charge transfer absorption     Simultaneous enectroscopy.		
	<ul><li>2. Simultaneous spectroscopy</li><li>3. Derivative Spectroscopy</li></ul>		
	3. Derivative spectroscopy		
3.2.2	Dual spectrometry – Introduction, Principle, Instrumentation and Applications		
3.3	Infrared Absorption Spectroscopy:	6 L	
3.3.1	Instrumentation: Sources, Sample handling, Transducers, Dispersive, non-		
	dispersive instrument		
3.3.2	FTIR and its advantages		
3.3.3	Applications of IR [Mid IR, Near IR, Far IR]: Qualitative with emphasis on		
	"Finger print" region, Quantitative analysis, Advantages and Limitations of IR		
3.3.4	Introduction and basic principles of diffuse reflectance spectroscopy.		
UNIT IV	THERMAL METHODS	15L	
4.1	Thermal methods:	9L	
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 crystallinity, oxidative stability, Drug analysis, Analysis of		
	Polyethylene for its crystallinity.		
4.2	Thermometric titrations:		
	Introduction, instrumentation, applications in the titration of (i) HCl Vs NaOH	<b>6</b> L	
	(ii) Boric acid Vs NaOH (iii) A mixture of Ca <sup>2+</sup> and Mg <sup>2+</sup> Vs EDTA (iv)		
	Zn <sup>2+</sup> with disodium tartarate.		
	REFERENCES		
	<ol> <li>Modern Analytical Chemistry by David Harvey, McGraw-Hill Higher Educe</li> <li>Principles of Instrumental Analysis - Skoog, Holler and Nieman, 5<sup>th</sup> Edition</li> </ol>		
	3. Fundamentals of Analytical Chemistry, By Douglas A. Skoog, Donald M.		
	James Holler, Stanley R. Crouch, 9 <sup>th</sup> Edition, 2004, Ch: 5.  4. Undergraduate Instrumental Analysis, 6 <sup>th</sup> Edition, J W Robinson, Marcel Dekker,		
UNIT I	Ch:1.	,	
	5. ISO 9000 Quality Systems Handbook, Fourth Edition, David Hoyle. (Cha	pter: 3 &	
	4) (Free download).	-	
	6. Quality in the Analytical Laboratory, Elizabeth Prichard, Wiley India, Ch. 5, Ch. 6 &Ch. 7		
	7. Quality Control and Total Quality Management - P.L. Jain-Tata McC	iraw-Hill	
	,. Quanty control and four Quanty Management 1.D. Juni-Tata McC	J.W 11 11111	

	<ul> <li>(2006) Total Quality Management - Bester field - Pearson Education, Ch:5.</li> <li>8. OECD Principles of Good Laboratory Practice (as revised in 1997)". OECD Environmental Health and Safety Publications. OECD. 1. 1998.</li> </ul>
UNIT II	1. 3000 solved problems in chemistry, Schaum's Solved problem series, David E. Goldbers, McGraw Hill international Editions, Chapter 11,15,16,21,22
	<ol> <li>D. A. Skoog, F. J. Holler, T. A. Nieman, Principles of Instrumental Analysis, 5<sup>th</sup> Edition, Harcourt Asia Publisher. Chapter 6, 7.</li> <li>H. H. Willard, L. L. Merritt, J. A. Dean, F. A. Settle, Instrumental Methods of Analysis,6 th Edition, CBS Publisher. Chapter 2.</li> </ol>
UNIT III	<ol> <li>R. D. Braun, Introduction to Instrumental Analysis, McGraw Hill Publisher. Chapter 8.</li> <li>G. W. Ewing, Instrumental Methods of Chemical Analysis, 5 th Edition, McGraw</li> </ol>
	<ul> <li>Hill Publisher, Chapter 3.</li> <li>M. Ito, The effect of temperature on ultraviolet absorption spectra and its relation to hydrogen bonding, J. Mol. Spectrosc. 4 (1960) 106-124.</li> </ul>
UNIT IV	<ol> <li>Introduction to instrumental methods of analysis by Robert D. Braun, Mc. Graw Hill (1987): Chapter 27</li> <li>Thermal Analysis-theory and applications by R. T. Sane, Ghadge, Quest Publications</li> <li>Instrumental methods of analysis, 7 th Edition, Willard, Merrit, Dean: Chapter 25</li> <li>Instrumental Analysis, 5 th Edition, Skoog, Holler and Nieman: Chapter 31</li> <li>Quantitative Chemical Analysis, 6 th Edition, Vogel: Chapter 12</li> <li>Analytical Chemistry by Open Learning: Thermal Methods by James W. Dodd &amp; Edition, Kenneth H. Tonge</li> </ol>

NAME OF THE COURSE	ANALYTICAL CHEM	ISTRY 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 determine percentage composition of saline injection. Estimation of sodium chloride by Volhard's method and glucose by polarimetry.
	2. To determine (a) the ion exchange capacity (b) exchange efficiency of the given cation exchange resin.
3	To determine the amount of Cr(III) and Fe(II) individually in a mixture of the two by titration with EDTA.
	To determine the breakthrough capacity of a cation exchange resin.
5	5. To determine the amount of Cu(II) present in the given solution containing a mixture of Cu(II) and Fe(II).
	5. To estimate Vitamin B <sub>12</sub> /fluorescein by fluorimetry.
	7. Simultaneous determination of Cr(VI) and Mn(VII) in a mixture spectrophotometrically

### **References:**

- 1. Quantitative Inorganic Analysis including Elementary Instrumental Analysis by A. I. Vogel's, 3<sup>rd</sup> 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, 4<sup>th</sup> Ed., A Wiley Interscience Publication, 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	<b>EXAMINATION</b>
TOTAL MARKS	50	50
PASSING MARKS	20	20

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 1	CHEMICAL THERMODYNAMICS – II	15L	
1.1	Fugacity of real gases - Determination of fugacity of real gases using graphical		
1.1	method and from equation of state. Equilibrium constant for real gases in terms of		
	fugacity. Gibbs energy of mixing, entropy and enthalpy of mixing.		
Real solutions- Partial molal quantities, partial molal volume, Gibbs Duhem			
1.2	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	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 translational and potential, separation of variables, the R the $\theta$ * and the $\phi$ 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 3	CHEMICAL KINETICS AND MOLECULAR REACTION DYNAMICS	15L
3.1	General Catalytic Mechanisms – Equilibrium treatment, steady state treatment, Activation energies for catalyzed reactions 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 4	SOLID STATE CHEMISTRY AND PHASE EQUILIBRIA	15L
4.1	Solid State Chemistry	
4.1.1	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 and 19)	
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.	
	III. Solid liquid Equilibria - Ternary solutions with common ions – (NaCl – KCl-	
	H <sub>2</sub> O and NaCl- Na <sub>4</sub> SO <sub>4</sub> - H <sub>2</sub> O)	
	(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.
- 3. Robert J. Silby and Robert A. Alberty, Physical Chemistry, 3rd Edition, John Wiley and Sons (Asia) Pte. Ltd., 2002.
- 4. Ira R. Levine, Physical Chemistry, 5<sup>th</sup> Edition, Tata McGraw-Hill New Delhi, 2002.
- S. Glasstone, Text Book of Physical Chemistry, 2ndEdition., McMillan and Co. Ltd., London, 1962.
- 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.
- 10. Peter A. Rock, Chemical Thermodynamics, University Science Books, Oxford University Press, 1983.
- 11. Thomas Engel and Philip Reid, Physical Chemistry, 3<sup>rd</sup> 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
NNon	– 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.
Instru	mental:
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, 3<sup>rd</sup> 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 CHEMISTRY		
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	
1.1	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).	
1.2	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)	5L

	1.) C 1 1 1 1 1 1 1 1 1 1 1 1 1 1		
	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 mechanisms, complimentary and non-complimentary reactions.		
1.4	Stereochemistry of substitution reactions of octahedral complexes. (Isomerization and racemization reactions and applications.)		
UNIT 2	ORGANOMETALLIC CHEMISTRY OF TRANSITION METALS	15L	
2.1	Eighteen and sixteen electron rule comparison and electron counting with examples.		
2.2	Preparation 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	10L	
2.2	(d) Alkyne derivatives of Pd and Pt  (e) Allyl derivatives of nickel  (f) Sandwich compounds of Cr and Half Sandwich compounds of Cr, Mo.  Structure and bonding on the basis of VBT and MOT in the following organometallic compounds:		
2.3	Zeise's salt, bis(triphenylphosphine)diphenylacetylene platinum(0) [Pt(PPh <sub>3</sub> ) <sub>2</sub> (HC≡CPh) <sub>2</sub> ], diallyl nickel(II), ferrocene and bis(arene)chromium(0), tricarbonyl (η²-butadiene) iron(0).		
UNIT 3	ENVIRONMENTAL CHEMISTRY	15L	
3.1	Introduction and discussion of toxicity of Heavy Metals:Toxicity of metallic 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  (a) Itai-itai disease for Cadmium toxicity,  (b) Arsenic Poisoning in the Indo-Bangladesh region.  (Other relevant examples recent may be included)		
3.2	Interaction of radiation in context with the environment:Sources and 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 4	BIOINORGANIC CHEMISTRY		
4.1	Biological oxygen carriers- heme and non heme: hemoglobin, hemerythrene and hemocyanin- structure of metal active center and differences in 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	3L	

4.3	Nitrogen fixation-nitrogenase, hydrogenases	3L			
4.4	Metal ion transport and storage: Ionophores and metallothionins				
	REFERENCES				
UNIT I	<ol> <li>P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Inorganic Chemistry, 5<sup>th</sup> Ed., Oxford University Press, 2010.</li> <li>W. H. Malik, G. D. Tuli and R. D. Madan, Selected Topics in Inorganic Chemistry, 8<sup>th</sup> Ed., S. Chand &amp; Company ltd.</li> <li>M. L. Tobe and J. Burgess, Inorganic Reaction Mechanism, Longman, 1999.</li> <li>S. Asperger, Chemical kinetics and Inorganic Reaction Mechanism, 2nd Ed., Kluwer Academic/ Plenum Publishers, 2002</li> <li>F. Basalo and R. G. Pearson, Mechanism of Inorganic Reactions, 2nd Ed., Wiley, 1967.</li> <li>R. Gopalan and V. Ramlingam, Concise Coordination chemistry, Vikas Publishing house Pvt Ltd., 2001.</li> <li>Robert B. Jordan, Reaction Mechanisms of Inorganic and Organometallic Systems, 3<sup>rd</sup> Ed., Oxford University Press 2008.</li> </ol>				
UNIT II	<ol> <li>D. Banerjea, Coordination chemistry. Tata McGrew Hill, New Delhi,1993.</li> <li>R.C Mehrotra and A.Singh, Organometallic Chemistry- A unified Approach, 2nded, New Age International Pvt Ltd, 2000.</li> <li>R.H Crabtree, The Organometallic Chemistry of the Transition Metals, 5th edition, Wiley International Pvt, Ltd 2000.</li> <li>B.Doughlas, D.H McDaniel and J.J Alexander. Concepts and Models of Inorganic Chemistry, 2<sup>nd</sup> edition, John Wiley and Sons. 1983.</li> <li>Organometallic Chemistry by G.S Sodhi. Ane Books Pvt Ltd.</li> </ol>				
UNIT	<ol> <li>Environmental Chemistry 5th edition, Colin Baird Michael Cann, W. H. Freeman and Company, New York, 2012.</li> <li>Environmental Chemistry 7th edition, Stanley E. Manahan, CRC Press Publishers,</li> <li>Environmental Contaminants, Daniel A. Vallero, ISBN: 0-12-710057-1, Elsevier Inc., 2004.</li> <li>Environmental Science 13th edition, G. Tyler Miller Jr. and Scott E. Spoolman, ISBN100-495-56016-2, Brooks/Cole, Cengage Learning, 2010.</li> <li>Fundamentals of Environmental and Toxicological Chemistry 4th edition, Stanley E. Manahan, ISBN: 978-1-4665-5317-0, CRC Press Taylor &amp; Francis Group, 2013.</li> <li>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</li> </ol>				
UNIT	<ol> <li>R. W. Hay, Bioinorganic Chemistry, Ellis Harwood, England, 1984.</li> <li>I. Bertini, H.B.Gray, S. J. Lippard and J.S. Valentine, Bioinorganic Chemistry, First South Indian Edition, Viva Books, New Delhi, 1998.</li> <li>J. A. Cowan, Inorganic Biochemistry-An introduction, VCH Publication, 1993.</li> <li>S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Publications, Mill Valley, Caligronic, 1994.</li> </ol>				

- 5. G.N. Mukherjee and A. Das, Elements of Bioinorganic Chemistry, Dhuri& Sons, Calcutta, 1988.
- 6. J.Chem. Educ. (Special issue), Nov, 1985.
- 7. E.Frienden, J.Chem. Educ., 1985, 62.
- 8. Robert R.Crechton, Biological Inorganic Chemistry An Introduction, Elsevier

NAME OF THE COURSE	INORGANIC CHEMIS	TRY 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)
I] Inorganic Preparations (Synthesis and Characterization) 1) Bis-(tetraethylammonium) tetrachloroCuprate (II) (Et <sub>4</sub> N) <sub>2</sub> [CuCl <sub>4</sub> ]
2) Bis-(tetraethylammonium)tetrachloroNickelate(II) (Et <sub>4</sub> N) <sub>2</sub> [NiCl <sub>4</sub> ] 3) Tetramminemonocarbanato Cobalt (III) Nitrate [Co(NH <sub>3</sub> ) <sub>4</sub> CO <sub>3</sub> ]NO3
4) Hydronium dichlorobis( dimethylglyoximato) Cobaltate(III) H[Co(dmgH) <sub>2</sub> Cl <sub>2</sub> ]

5) Bis (ethylenediammine) Copper (II) Sulphate [Cu(en)<sub>2</sub>]SO<sub>4</sub>

#### II] Instrumentation

- 1) Determination of equilibrium constant by Slope intercept method for Fe<sup>+3</sup>/ 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

#### **REFERENCES**

- 1. Advanced experiments in Inorganic Chemistry., G. N. Mukherjee., 1<sup>st</sup> Edition., 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

NAME OF THE COURSE	ORGANIC CHEMISTR	RY
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 1	ALKYLATION AND REACTION OF CARBON NUCLEOPHILES		
1.1	Alkylation of Nucleophilic Carbon Intermediates:		
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		
115	enamines and imines.		
1.1.5	Alkylation of carbon nucleophiles by conjugate addition (Michael reaction).	8L	
	Reaction of carbon nucleophiles with carbonyl groups	δL	
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. Claisen reaction, Perkin Reformatsky Darzens, Knoevenagel reaction.		
1.2.2	Addition reactions with amines and iminium ions; Mannich reaction.		
1.2.2	Acylation of carbanions.		
1.2.3	Acylation of Carbanions.		
	[Reference Books: 1-11]		
UNIT 2	REACTIONS AND REARRANGEMENTS	15L	
	Mechanisms, stereochemistry (if applicable) and applications of the following:		
2.1	<b>Reactions:</b> Baylis-Hilman reaction, McMurry Coupling, Corey-Fuchs reaction, Nef reaction, Passerini reaction. Wittig		
2.2	Concerted rearrangements: Hofmann, Curtius, Lossen, Schmidt, Wolff, BoultonKatritzky.		
2.3	Cationic rearrangements: Tiffeneau-Demjanov, Pummerer, Dienone-phenol, Rupe, Wagner-Meerwein.		
2.4	<b>Anionic rearrangements:</b> Brook, Neber, Von Richter, Wittig, Gabriel-Colman, Payne.		
-	[Reference Books: 19-22]		
UNIT 3	MOLECULAR ORBITAL THEORY		
3.1	Introduction to Molecular Orbital Theory for Organic Chemistry:	<b>8</b> L	
3.1.1	<b>Molecular orbitals:</b> Formation of $\sigma$ - and $\pi$ -MOs by using LCAO method.		
	Formation of $\pi$ MOs of ethylene, butadiene, 1, 3, 5-hexatriene,. Concept of nodal planes and energies of $\pi$ -MOs		
3.1.2	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 allylcation with allyl		
3.1.3	anion.		
	<b>MOs of formaldehyde:</b> The effect of electronegativity perturbation and orbital polarization in formaldehyde. HOMO and LUMO ( $\pi$ and $\pi^*$ orbitals) of		

3.1.4 3.1.5 3.2 3.2.1 3.2.2 3.2.3 3.2.4 3.2.5	formaldehyde. Perturbation Theory of Reactivity. Addition of hydride to formaldehyde.  The Salem-Klopman equation. (no derivation and no remembrance of the equation) 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.  Application of FMO concepts in (a) S <sub>N</sub> <sup>2</sup> reaction, (b) ethylene dimerization to cyclobutane (c) Diels-Alder cycloaddition.  Photochemistry:  General Principles  Orbital Symmetry Considerations for Photochemical Reactions of Alkenes and Dienes, Photochemical Electrocyclic Reactions  Photochemical cross coupling of alkenes. Photo dimerisation of alkenes.  Photochemistry of arenes 1,2; 1,3 and 1,4 addition photocycloaddition of aromatic rings.	7L
3.2.6	Photochemically induced radical reactions. Chemiluminiscence	
UNIT 4	SPECTROSCOPY	15L
4.1	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).	3L
4.2	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.	4L
4.3	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.  13C 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	4L

	and carbonyl carbons.	
	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	
4.4	compounds (including compounds containing hetero atoms), McLafferty	4L
	rearrangement, Retro-Diels-Alder reaction.	
	Structure determination involving individual or combined use of the above	
	spectral techniques.	
	[Reference Books: 13-18]	

#### REFERENCES

- 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 (7<sup>th</sup> 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, 6<sup>th</sup> Edition.
- 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 CHEMISTE	RY 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	4 To elucidate the structure of a compound based on spectra	

ORGANIC CHEMISTRY PRACTICAL	
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:
  - (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.

I. Identification of a compound based on spectral interpretation of data of IR <sup>1</sup>H and <sup>13</sup>C NMR and mass spectrum

#### **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
	Concept of plate and rate theories in chromatography: efficiency, resolution,	4L
1.1	selectivity and separation capability. Van Deemter equation and broadening of	
	chromatographic peaks. Optimization of chromatographic conditions.	
	Gas Chromatography:	
1.2	Instrumentation of GC with special reference to sample injection systems –	3L
1.2	split/splitless, column types, solid/ liquid stationary phases, column switching	
	techniques, temperature programming, Thermionic and mass spectrometric detector,	
	Applications.	
	HPTLC:	
1.3	Introduction to HPTLC, techniques in HPTLC. Determination by detectors: single	5L
	beam densitometer, double beam densitometer, fluorimetric detector. Comparison	
	between TLC and HPTLC. Advantages, limitations and applications of HPTLC	
1.4	Size exclusion chromatography:	
1.4	Basic principle and applications in the field of polymers	3L
UNIT 2	SPECTROMETRY AND RADIO-ANALYTICAL METHODS	15L
0.1	X-ray spectroscopy:	4L
2.1	Principle, instrumentation and applications of X-ray fluorescence, absorption and	
	diffraction spectroscopy.	
	Mass spectrometry:	
	Recapitulation, instrumentation, ion sources for molecular studies, electron impact,	6L
2.2	field	
	ionization, field desorption, chemical ionization and fast atom bombardment sources.	
	Mass analyzers: Quadrupole, time of flight and ion trap. Applications.	

	Dadie analytical Mathada	
2.3	Radio analytical Methods:  Recapitulation, isotope dilution method, introduction, principle, single dilution method, double dilution method and applications.	5L
UNIT III	SURFACE ANALYTICAL TECHNIQUES	15L
3.1	Surface Analytical Techniques: Introduction, Principle, Instrumentation and Applications of:	9L
3.1.1	Scanning Electron Microscopy (SEM)	
3.1.2	Scanning Tunnelling 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.	
UNIT IV	ELECTROANALYTICAL METHODS	15L
4.1	Ion selective potentiometry and Polarography:	10L
4.1.1	Ion selective potentiometry:	TOL
4.1.2	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.	2L
	REFERENCES	
UNIT I	Instrumental Analysis, Skoog, Holler & Erouch     HPTLC Analysis: Dilip Charegaonkar	
UNIT II	<ol> <li>Essentials of Nuclear Chemistry, H J Arnikar, New Age Publishers (2005)</li> <li>Fundamentals of Radiochemistry D. D. Sood, A. V. R. Reddy and N. Ramamoorthy</li> <li>Principles of Instrumental Analysis - Skoog, Holler and Nieman, 5<sup>th</sup> Edition, Ch: 12</li> </ol>	
UNIT III	<ol> <li>Physical Principles of Electron Microscopy, An Introduction to TEM, SEM, and AE</li> <li>Authors: Ray F. Egerton, ISBN: 978-0- 387-25800- 3 (Print) 978-0- 387-26016- 7 (</li> <li>Modern techniques of surface science by D.P. Woodruff, T.A. Delchar, Cambridge Press, 1994.</li> </ol>	Online)

	<ol> <li>Introduction to Scanning Tunneling Microscopy by C. J. Chen, Oxford University Press, NewYork, 1993.</li> <li>Transmission Electron Microscopy: A text book for Material Science, David B Williams and C., Barry Carter, Springer</li> <li>Modern Spectroscopy, by J.M. Hollas, 3rd Edition (1996), John Wiley, New York</li> <li>Principles of Instrumental Analysis – Skoog, Holler, Nieman, 5th ed., Harcourt College</li> </ol>
	Publishers, 1998.
UNIT	<ol> <li>Principles of Instrumental Analysis – Skoog, Holler, Nieman, 5th Edition, Harcourt College Publishers, 1998. Chapters - 23, 24, 25.</li> <li>Modern Analytical Chemistry David Harvey; McGraw Hill Higher education publishers, (2000).</li> <li>Vogel's Textbook of quantitative chemical analysis, 6th edition, Pearson Education Limited, (2007).</li> <li>Electrochemical Methods Fundamentals and Applications, Allen J Bard and Larry R Faulkner, John Wiley and Sons, (1980).</li> <li>Instrumental Methods of Analysis Willard, Merrit, Dean and Settle, 7th edition, CBS publishers.</li> </ol>

NAME OF THE COURSE	ANALYTICAL CHEMISTRY 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 the amount of Ti (III) and Fe(II) in a mixture by titration with Ce(IV) potentiometrically.	
2.	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.	
3.	To determine the amount of Fe(II) and Fe(III) in a mixture using 1,10-phenanthroline spectrophotometrically.	
4.	To determine the percentage composition of HCl and H <sub>2</sub> SO <sub>4</sub> on weight basis in a mixture of two by conductometric titration with NaOH and BaCl <sub>2</sub> .	
5.	Demonstration separation of test dyes/ Separation and identification of a marker compound in a herbal formulation using HPTLC.	
6.	Simultaneous determination of Cd <sup>2+</sup> and Zn <sup>2+</sup> in an industrial effluent sample using calibration curve method polarographically.	
7.	To determine the amount of calcium in milk powder by flame photometry.	

### **REFERENCES**

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

# ASSESSMENT DETAILS: (for all the theory papers)

### **Internal Assessment (50 marks)**

Two tests of 25 marks each Activity of 25 maks Activities could be Test/ assignment/ project

Best two to be considered

### **Semester End Examination – External Assessment (50 marks)**

### Unit 1

Q1 Answer any two out of four [5 x 2=10]

Unit 2

Q2 Answer any two out of four [5 x 2=10]

Unit 3

Q3 Answer any two out of four [5 x 2=10]

### Unit 4

Q4 Answer any two out of four  $[5 \times 2=10]$ 

Unit 5

Q5 Answer any two out of four  $[5 \times 2=10]$ 

(One question from each Unit)

### **Practical Assessment (for papers with practicals)**

Practical examination of each paper for 50 marks will be held for three and half hours

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