

# University of Mumbai



M.Sc. Analytical Chemistry  
Semester I & II  
**CHOICE BASED (REVISED  
SYLLABUS) as per NEP 2020**  
with effect from the  
academic year  
2023–2024

**S.Z.S.P. Mandal's  
Shri Pancham Khemraj Mahavidhyalay,  
Sawantwadi416510  
(Autonomous)  
Affiliated to Mumbai university**

Sr. No.	Heading	Particulars
1	Title of the Course	<b>M.Sc. Analytical Chemistry</b>
2	Eligibility for Admission	B.Sc. Chemistry or equivalent qualification from other universities as may have been allowed by the relevant ordinances of this university
3	Passing Marks	40%
4	Ordinances / Regulations (if any)	
5	No. of Years /Semesters	Two
6	Level	PG
7	Pattern	Semester
8	Status	Revised
9	To be implemented from Academic Year	From Academic Year: 2023-2024

Date:

Signature:

Chairman BoS in Chemistry

Dean, Science and Technology

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**Credit Distribution Structure for Two Years**  
**(M.Sc. in Analytical Chemistry)**

Year	Level	Sem	Major				RM	OJT/FP	RP	Cum. Cr.	Degree	
			Mandatory			Electives						
1	6.0	Sem I	3*4+ 2=14			4	4	Research Methodology (CHEM 506)		-	22	PG Diploma (after 3 Years Degree)
			Inorganic Chemistry-I (CHEM 501)	TH	4	<b>Credits 4 (2+2)</b> <b>Course 1 :</b> Physical Chemistry-I + Chemistry Practicals (Inorganic Chemistry and Physical Chemistry) (CHEM 50211)  <b>(OR)</b> <b>Credits 4 (2+2)</b> <b>Course 2 :</b> Physical Chemistry-II + Chemistry Practicals (Inorganic Chemistry and Physical Chemistry) (CHEM 50212)						
			Organic Chemistry-I (CHEM 503)	TH	4							
			Analytical Chemistry-I (CHEM 505)	TH	4							
		Chemistry Practical-I (Analytical Chemistry and Organic Chemistry) (PRCHEMAP 504)	PR	2								
		Sem II	3*4+ 2=14			4	-	4	-	22		
			Inorganic Chemistry-II (CHEM 507)	TH	4	<b>Credits 4 (2+2)</b> <b>Course 1 :</b> Physical Chemistry-III + Chemistry Practicals (Inorganic Chemistry and Physical Chemistry) (CHEM 50811)  <b>(OR)</b> <b>Credits 4 (2+2)</b> <b>Course 2 :</b> Physical Chemistry-IV + Chemistry Practicals (Inorganic Chemistry and Physical Chemistry) (CHEM 50812)						
			Organic Chemistry -II (CHEM 509)	TH	4							
Analytical Chemistry -II (CHEM 510)	TH		4									
Chemistry Practical-II (Analytical Chemistry and Organic Chemistry) (PRCHEMAP 511)	PR	2										
Cum. Cr. For PG Diploma			28	8	4	4		44				

Exit Option: PG Diploma (44 credits) after Three Year UG Degree

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**Syllabus for Approval**  
**Proposed Draft Syllabus For M.Sc. Analytical Chemistry Semester I and II**  
**Choice Based Credit System**  
**Under New Education Policy (NEP) 2020**  
**(To be implemented from the academic year, 2023-2024)**  
**PROGRAM OUTLINE 2023-2024**

YEAR		COURSE CODE	COURSE TITLE	CREDITS
M.Sc. Sem-I	Mandatory Course-I	CHEM 501	Inorganic Chemistry-I	04
	Mandatory Course-II	CHEM 503	Organic Chemistry-I	04
	Mandatory Course-III	CHEM 505	Analytical Chemistry-I	04
	Mandatory Course Practical	PRCHEMAP 504	Chemistry Practical-I (Analytical Chemistry and Organic Chemistry)	02
	Elective 1	CHEM 50211	Physical Chemistry-I and Chemistry Practical (Inorganic Chemistry and Physical Chemistry)	04
	Elective 2	CHEM 50212	Physical Chemistry-II and Chemistry Practical (Inorganic Chemistry and Physical Chemistry)	04
	RM	CHEM 506	Research Methodology	04
M.Sc. Sem-II	Mandatory Course-I	CHEM 507	Inorganic Chemistry-II	04
	Mandatory Course-II	CHEM 509	Organic Chemistry-II	04
	Mandatory Course-III	CHEM 510	Analytical Chemistry-II	04
	Mandatory Course Practical	PRCHEMAP 511	Chemistry Practical-II (Analytical Chemistry and Organic Chemistry)	02

	Elective 1	CHEM 50811	Physical Chemistry-III and Chemistry Practical (Inorganic Chemistry and Physical Chemistry)	04
	Elective 2	CHEM 50812	Physical Chemistry-IV and Chemistry Practical (Inorganic Chemistry and Physical Chemistry)	04
	OJT/FP	CHEM 512	Industrial Training/Field Project	04

**PROGRAMME SPECIFIC OUTCOME (PSOs) :**

1. To gain knowledge in chemistry, scrutinize and accomplish solution to problems encountered in the field of research and analysis.
2. To apply the basic knowledge of chemistry to perform various tasks at the workplace to meet global standards.
3. To deduce qualitative and quantitative information using various analytical techniques
4. To inculcate the aptitude of scientific approach along with analytical reasoning in technologies used in the Industry.
5. To explicit subject knowledge and integrate it in interdisciplinary research .
6. To understand, manage and contribute to solve societal and environmental issues ethically .
7. To exhibit professional work ethics and norms of scientific developments.
8. To develop critical thinking approach toward the scientific problems, analysis, validation and documentation with safety norms and standards.
9. To inculcate analytical thinking,so that students will have an edge for a better future in chemical industries.
10. To imbibe an attitude of lifelong learning so as to thrive in knowledge and skills.

<b>PROGRAM(s): M.Sc.-I</b>		<b>SEMESTER: I</b>			
<b>Course:</b> Mandatory Course-I		<b>Course Code: (CHEM 501)</b>			
		<b>Course Title: -Inorganic Chemistry-I</b>			
<b>Teaching Scheme</b>					<b>Evaluation Scheme</b>
<b>Lectures (Hours per week)</b>	<b>Practical (Hours per week)</b>	<b>Tutorial (Hours per week)</b>	<b>Credit</b>	<b>Continuous Assessment (CA) (Marks- 50)</b>	<b>Semester End Examination (Marks- 50)</b>
<b>04</b>	<b>NA</b>	<b>-</b>	<b>04</b>	<b>50</b>	<b>50</b>
<p><b>Learning Objectives:</b></p> <p><b>Inorganic Chemistry:</b></p> <ol style="list-style-type: none"> <li>1. To understand the concept of wave mechanics applicable to derive wave functions in hybridization, and applications of MOT to polyatomic species.</li> <li>2. To gain knowledge of molecular symmetry, group theory and its applications in order to elucidate structures of molecules.</li> <li>3. To have in depth knowledge of fundamentals of wave mechanics applicable to study electrical conductivity of solids</li> <li>4. To learn structural aspects of inorganic compounds</li> <li>5. To have awareness about cutting age topic like solid state lasers having wide commercial applications</li> <li>5. To enable the spectroscopic methods of characterization of inorganic compounds</li> <li>6. To develop the ability to solve numerical expressions using instrumental techniques.</li> </ol>					
<p><b>Course Outcomes:</b></p> <ol style="list-style-type: none"> <li>1) The learner will be able to express the derivations of wave equation and concept of MOT applied to diatomic &amp; polyatomic molecules.</li> <li>2). elucidate the structures of inorganic compounds and know the wide applications of solid state lasers.</li> <li>3). represent schematically Orgel and Tanabe Sugano diagrams, splitting of terms in octahedral environment.</li> </ol>					

**Semester – I**  
**Inorganic Chemistry-I**  
**(CHEM501)**

<b>Course code- CHEM 501</b>	<b>Unit</b>	<b>Course/Unit Title: Inorganic Chemistry-I</b>	<b>Credits 04/ [60 L]</b>
	1	<b>Chemical Bonding</b>	<b>[15L]</b>
		<p>1.1 Recapitulation of hybridization Derivation of wave functions for <math>sp</math>, <math>sp^2</math>, <math>sp^3</math> orbital hybridization types considering only sigma bonding.</p> <p>1.2 Discussion of involvement of d orbitals in various types of hybridizations.            Concept of resonance, resonance energy derivation expected. Formal charge with examples.</p> <p>1.3 Molecular Orbital Theory for diatomic species of First transition Series.</p> <p>1.4 Molecular Orbital Theory for Polyatomic species considering <math>\sigma</math> bonding for <math>SF_6</math>, <math>CO_2</math>, <math>B_2H_6</math>, <math>I_3^-</math> molecular species.</p> <p>1.5 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.</p>	

	2	<b>Molecular Symmetry and Group Theory</b>	[15L]
		<p>2.1. Symmetry criterion of optical activity, symmetry restrictions on dipole moment. A systematic procedure for symmetry classification of molecules.</p> <p>2.2. Concepts of Groups, Sub-groups, Classes of Symmetry operations, Group Multiplication Tables. Abelian and non-Abelian point groups.</p> <p>2.3.a) 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 <math>C_{2v}</math>, <math>C_{3v}</math> and <math>C_{2h}</math> structure of character tables.</p> <p>b) Determination of symmetry species for translations and rotations.</p> <p>c) Mulliken's notations for irreducible representations.</p> <p>d) Reduction of reducible representations using reduction formula.</p> <p>2.4. Applications of Group Theory Symmetry adapted linear combinations (SALC), symmetry aspects of MO theory, sigma bonding in <math>AB_n</math> (<math>NH_3</math>, <math>CH_4</math>) molecules.</p>	
	3	<b>Material Chemistry and Nanomaterials</b>	[15L]
		<p><b>3.1 Solid State Chemistry</b></p> <p>3.1.1. Electronic structure of solids and band theory, Fermi level, K Space and Brillouin Zones.</p> <p>3.1.2. Structures of Compounds of the type: AB [nickel arsenide (<math>NiAs</math>)], <math>AB_2</math> [fluorite (<math>CaF_2</math>) and anti-fluorite structures, rutile (<math>TiO_2</math>)</p> <p>3.1.3. Solid state lasers: Introduction, types, working and Applications</p>	



		<p><b>3.2 Nanomaterials</b></p> <p>3.2.1 Preparative methods, Chemical methods, solvothermal, combustion synthesis, microwave, coprecipitation, Langmuir-Blodgett(LB) method, biological methods, synthesis using microorganism.</p> <p>3.2.2 Applications in the field of semiconductors, solar cells.</p>	
	<b>4</b>	<b>Characterization of Coordination Compound</b>	<b>[15L]</b>
		<p>4.1. Methods of Characterization: thermal studies, Conductivity measurements, electronic spectral and magnetic measurements, IR, NMR and ESR spectroscopic methods.</p> <p>4.2. Introduction to Orgel &amp; Tanabe Sugano Diagram, Terms, Splitting of terms in Octahedral environment, Calculation of electron parameters such as <math>\Delta</math>, <math>B'</math>, <math>C</math>, Nephelauxetic ratio with suitable examples.</p> <p>4.3. Determination of formation constants of metal complexes (Overall and Stepwise): Comparative studies of Potentiometric and spectrophotometric method.</p>	

### References:

#### Unit- I

1. B. R. Puri, L. R. Sharma and K. C. Kalia, Principles of Inorganic Chemistry, Milestone Publishers, 2013-2014.
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, 4th Ed., Harper Collins, 1993.
6. P. J. Durrant and B. Durrant, Introduction to Advanced Inorganic Chemistry, Oxford University Press, 1967.
7. R. L. Dekock and H.B.Gray, Chemical Structure and Bonding, The Benjamin Cummings Publishing Company, 1989.
8. G. Miessler and D. Tarr, Inorganic Chemistry, 3rd Ed., Pearson Education, 2004.
9. R. Sarkar, General and Inorganic Chemistry, Books & Allied (P) Ltd., 2001.

10. C. M. Day and J. Selbin, Theoretical Inorganic Chemistry, Affiliated East West Press Pvt. Ltd., 1985.
11. J. N. Murrell, S. F. A. Kettle and J. M. Tedder, The Chemical Bond, Wiley, 1978.
12. G. A. Jeffrey, An Introduction to Hydrogen Bonding, Oxford University Press, Inc., 1997.

### Unit-II

1. F. A. Cotton, Chemical Applications of Group Theory, 2nd Edition, Wiley Eastern Ltd., 1989.
2. H. H. Jaffe and M. Orchin, Symmetry in Chemistry, John Wiley & Sons, New York, 1996.
3. R. L. Carter, Molecular Symmetry and Group Theory, John Wiley & Sons, New York, 1998.
4. K. V. Reddy. Symmetry and Spectroscopy of Molecules, 2nd Edition, New Age International Publishers, New Delhi, 2009.
5. A. Salahuddin Kunju and G. Krishnan, Group Theory and its Applications in Chemistry, PHI Learning, 2012.
6. P. K. Bhattacharya, Group Theory and its Chemical Applications, Himalaya Publishing House. 2014.
7. S. Swarnalakshmi, T. Saroja and R. M. Ezhilarasi, A Simple Approach to Group Theory in Chemistry, Universities Press, 2008.

### Unit-III

1. Solid State Chemistry Introduction, Lesley E. Smart, Elaine A. Moore, ISBN 0- 203-49635-3, 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. Rao, A. Muller, and A.K. Cheetham, ISBN 978-3-527-31664-9, 2007 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.
7. Peter Atkins and Julio de Paula, Atkin's *Physical Chemistry*, 7<sup>th</sup> Edn., Oxford University Press, 2002.
8. An introduction to Lasers Theory and Applications by M.N. Avadhanulu. P.S.Hemne, S. Chand publications.
9. Advances in solid state lasers development and Applications by M.Grishin.
10. Solid State Lasers \_ A graduate Text by Walter Koechner, Michael Bass, Springer.
11. Rare earth materials – properties and applications by A,R.Jha, CRC Press.

### Unit IV

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 Tata McGraw Hill 1993

3. Geary Coordination reviews 4. P.W. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong; Shriver & 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 edn.), John Wiley & Sons (1994).

<b>PROGRAM(s): M.Sc.-I</b>		<b>SEMESTER: I</b>			
<b>Course: Mandatory Course-II</b>		<b>Course Code: (CHEM503)</b>			
		<b>Course Title: - Organic Chemistry-I</b>			
<b>Teaching Scheme</b>					<b>Evaluation Scheme</b>
<b>Lectures (Hours per week)</b>	<b>Practical (Hours per week)</b>	<b>Tutorial (Hours per week)</b>	<b>Credit</b>	<b>Continuous Assessment (CA) (Marks- 50)</b>	<b>Semester End Examination (Marks- 50)</b>
<b>04</b>	<b>NA</b>	<b>--</b>	<b>04</b>	<b>50</b>	<b>50</b>
<b>Learning Objectives:</b>					
<p>1.To enable learners to have comprehensive knowledge and understanding of the advanced concepts in reaction Mechanism, stereochemistry, different reactions and reagents.</p> <p>2. To apply the basic knowledge of Organic chemistry to perform various tasks assigned to them at the workplace in industry and academia to meet the job requirements as per global standards.</p> <p>3. Accomplish a solution to problems encountered in the field of research.</p>					
<b>Course Outcomes.</b>					
After completing the course students will be able to:					
1) predict the reactivity of organic compound from its structure.					

- 2) understand different methods used for determination of Organic Reaction Mechanism
- 3) understand the fundamental concept in stereochemistry by applying various symmetry elements of organic molecule.
- 4) acquire the knowledge of chirality by taking examples of symmetrical and unsymmetrical molecule.
- 5) develop interest in stereochemistry by studying stereochemical features of different classes of organic compounds
- 6) identify the nomenclature of various stereochemical phenomena
- 7) organize the techniques of aromatic nucleophilic substitution reactions for synthesizing/transforming molecules.
- 8) understand the concept of aromaticity and to know the nature of bonds, electronic effects and other properties of molecules.
- 9) understand the preparation of important oxidizing reagent and predict the selectivity of the reagents in organic reactions.
- 10) explain the preparation and uses of important reducing reagents in various organic transformation reaction.

Course Code: (CHEM 503)	Unit	Course Title: - Organic Chemistry-I	Credits:04 60L
	<b>1</b>	<b>Physical Organic Chemistry:</b>	<b>(15L)</b>
		<b>1.1.Thermodynamic and kinetic requirements of a reaction:</b> rate and equilibrium constants, reaction coordinate diagram, transition state (activated complex), nature of activated complex, Hammond postulate, Reactivity <i>vs</i> selectivity, Curtin-Hammett Principle, Microscopic reversibility, Kinetic <i>vs</i> thermodynamic control of organic reactions.	
		<b>1.2.Determining mechanism of a reaction:</b> 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.	
		<b>1.3.Acids and Bases:</b> 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.	
	<b>2</b>	<b>Stereochemistry</b>	<b>(15 L)</b>

		<b>2.1. Concept of Chirality:</b> Recognition of symmetry elements.	
		<b>2.2 Molecules with tri- and tetra-coordinate centers:</b> Compounds with carbon, silicon, nitrogen, phosphorous and sulphur chiral centers, relative configurational stabilities	
		<b>2.3. Molecules with two or more chiral centers:</b> 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 pseudoasymmetric centres. R-S nomenclature for chiral centres in acyclic and cyclic compounds.	
		<b>2.4. Axial and planar chirality:</b> 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.	
		<b>2.5. Prochirality:</b> 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 stereoheterotopic ligands and faces. Symbols for stereoheterotopic 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-pseudoasymmetric centre. Symbols for enantiotopic and diastereotopic face.	
	<b>3</b>	<b>Nucleophilic substitution reactions and Aromaticity</b>	<b>(15L)</b>
		<b>3.1 Nucleophilic substitution reactions. (9 L)</b> <b>3.1.1 Aliphatic nucleophilic substitution:</b> $S_N1$ , $S_N2$ , $S_Ni$ reactions, mixed $S_N1$ and $S_N2$ and SET mechanisms. $S_N$ reactions involving NGP - participation by aryl rings, $\sigma$ and pi-bonds. Factors affecting these reactions: substrate, nucleophilicity, solvent, steric effect, hard-soft interaction, leaving group. Ambident nucleophiles. $S_{NCA}$ , $S_N1''$ and $S_N2''$	

		<p>reactions. <math>S_N</math> at <math>sp^2</math> (vinylic) carbon.</p> <p><b>3.1.2 Aromatic nucleophilic substitution:</b> <math>S_NAr</math>, <math>S_N1</math>, benzyne mechanisms. Ipso, cine, tele and vicarious substitution.</p> <p><b>3.1.3 Ester hydrolysis:</b> Classification, nomenclature and study of all eight mechanisms of acid and base catalyzed hydrolysis with suitable examples.</p>	
		<p><b>3.2. Aromaticity (6 L)</b></p> <p>3.2.1. Huckel's <math>(4n+2)</math> and <math>4n</math> rules, structural, thermochemical, and magnetic criteria for aromaticity, including NMR characteristics of aromatic systems. Delocalization and aromaticity.</p> <p>3.2.2. Aromatic and antiaromatic compounds up-to 18 carbon atoms. Homoaromatic compounds. Aromaticity of all benzenoid systems, heterocycles, metallocenes, azulenes, annulenes, aromatic ions and Fullerene (<math>C_{60}</math>).</p>	
	<b>4</b>	<p><b>Oxidation and Reduction:</b></p> <p><b>4.1 Oxidation:</b> General mechanism, selectivity, and important applications of the following:</p> <p><b>4.1.1. Dehydrogenation:</b> Dehydrogenation of C-C bonds including aromatization of six membered rings using metal (Pt, Pd, Ni) and organic reagents (chloranil, DDQ).</p> <p><b>4.1.2. Oxidation of alcohols to aldehydes and ketones:</b> Chromium reagents such as <math>K_2Cr_2O_7/H_2SO_4</math> (Jones reagent), <math>CrO_3</math>-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.</p> <p><b>4.1.3. Oxidation involving C-C bonds cleavage:</b> Glycols using <math>HIO_4</math>; cycloalkanones using <math>CrO_3</math>; carbon-carbon double bond using ozone, <math>KMnO_4</math>, <math>CrO_3</math>, <math>NaIO_4</math> and <math>OsO_4</math>; aromatic rings using <math>RuO_4</math> and <math>NaIO_4</math>.</p> <p><b>4.1.4. Oxidation involving replacement of hydrogen by oxygen:</b> oxidation of <math>CH_2</math> to CO by <math>SeO_2</math>, oxidation of arylmethanes by <math>CrO_2Cl_2</math> (Etard oxidation).</p> <p><b>4.1.5. Oxidation of aldehydes and ketones:</b> with <math>H_2O_2</math> (Dakin reaction), with peroxy acid (Baeyer-Villiger oxidation)</p> <p><b>4.2 Reduction:</b> General mechanism, selectivity, and important applications of the following reducing reagents:</p> <p><b>4.2.1. Reduction of CO to <math>CH_2</math> in aldehydes and ketones-</b> Clemmensen reduction, Wolff-Kishner reduction and Huang-</p>	<b>(15L)</b>

	<p>Minlon modification.</p> <p><b>4.2.2. Metal hydride reduction:</b> 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).</p> <p><b>4.2.3.</b> N<sub>2</sub>H<sub>2</sub> (diimide reduction) and other non-metal-based agents including organic reducing agents (Hantzsch dihydropyridine).</p> <p><b>4.2.4. Dissolving metal reductions:</b> using Zn, Li, Na, and Mg under neutral and acidic conditions, Li/Na-liquid NH<sub>3</sub> mediated reduction of aromatic compounds (Birch reduction) and Alkynes.</p>	
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#### Reference Books.

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

- Press.
17. Organic Synthesis, Jagdamba Singh, L.D.S. Yadav, Pragati Prakashan.
  18. Modern Methods of Organic Synthesis, W. Carruthers and Iain Coldham, Cambridge University Press.
  19. Organic reactions and their Mechanisms, P.S. Kalsi, New Age International Publishers.
  20. Organic Synthesis, Jagdamba Singh, L.D.S Yadav, Pragati Prakashan.
  21. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Nelson Thornes

<b>PROGRAM(s): M.Sc.-I</b>				<b>SEMESTER: I</b>
<b>Course : Mandatory Course-III</b>				<b>Course Code: (CHEM 505)</b>
				<b>Course Title:-Analytical Chemistry-I</b>
<b>Teaching Scheme</b>				<b>Evaluation Scheme</b>
<b>Lectures (Hours per week)</b>	<b>Practical (Hours per week)</b>	<b>Credit</b>	<b>Continuous Assessment (CA) (Marks- 50)</b>	<b>Semester End Examination (Marks- 50)</b>
<b>04</b>	<b>NA</b>	<b>04</b>	<b>50</b>	<b>50</b>
<b>Learning Objectives:</b>				
<ol style="list-style-type: none"> <li>1. To enable learners to have comprehensive knowledge, understanding of the types of instruments with operations and automated methods of analysis.</li> <li>2. To apply the basic knowledge of quality systems, quality audit and quality managements.</li> <li>3. To enable learners to perform various tasks assigned to them at the workplace in industry and academia to meet the job requirements as per global standards.</li> <li>4. To provide solutions to problems encountered in the field of analysis and research.</li> </ol>				
<b>Course Outcomes:</b> After completion of this Course, the learner will be able to:				
<ol style="list-style-type: none"> <li>1. Understand various terms used in analytical chemistry.</li> <li>2. Identify the different types of errors in analysis.</li> <li>3. Sketch out the role and importance of total quality management, safety, accreditations</li> </ol>				



- and GLP in industries.
4. Understand the efficacy of automation in chemical analysis.
  5. Design and specify applications of advanced analytical techniques in various fields.
  6. Explore the applications of IR spectroscopy and thermal methods.
  7. Perform basic calculations required in chemical analysis.
  8. Interpret the experimental results of analytical techniques.

<b>Course code- CHEM 505</b>	<b>Unit</b>	<b>Course/Unit Title- Analytical Chemistry-I</b>	<b>Credits 04/ 60 Lectures</b>
	1	<b>Analytical Chemistry-I</b>	<b>[15L]</b>
		<p><b>1.1. Language of Analytical Chemistry</b></p> <p>1.1.1 Analytical perspective [3 L]</p> <p>Analytical approach. common analytical problems. Terms involved in analytical chemistry - Analysis, Analyte, Matrix, Determination, Measurement, Techniques, Methods, Procedures and protocol.</p> <p>1.1.2 An overview of analytical methods [3 L]</p> <p>Analytical methods - Types, classification and selection. Quantitative method of Analysis- Calibration method, Method of Standard addition, Internal standard method. Performance Characteristics of analytical method- Accuracy, Precision, Selectivity, Sensitivity, Detection limit (LOD, LOQ, LOL) ,Dynamic range and Robustness and Ruggedness.</p> <p>1.1.3 Errors [2 L]</p> <p>Types of errors. Absolute error, Relative error, Constant error and Proportionate errors. Minimization of errors.</p>	<b>[8 L]</b>

		<p><b>1.2 Quality in Analytical Chemistry</b></p> <p>1.2.1 Total Quality Management- TQM [3L]</p> <p>Definition, Principles, Importance and benefits. Philosophy of implementation of TQM -Process steps, Advantages and Limitations <b>i)</b> Kaizen -Six steps <b>ii)</b> Six Sigma approach <b>iii)</b> 5S and 5S audit check for laboratories.</p> <p>1.2.2 Safety in laboratories [2L]</p> <p>Basic concept of safety in laboratory- The Industrial Hygiene Principles. Personal protection equipment (PPE). Occupational Safety and Health Administration (OSHA).</p> <p>1.2.3 Accreditations [2L]</p> <p>Accreditation of laboratories, NABL, Indian Government standards (ISI, HALLMARK, AGMARK).- Meaning and significance.</p>	[7L]
	2.	<p><b>2.1 Calculations based on Chemical Principles</b></p> <p><i>(The following topics are to be covered in the form of numerical problems only)</i></p> <p>2.1.1 Concentration of a solution based on volume and mass units.</p> <p>2.1.2 Calculations of ppm, ppb and dilution of the solutions, concept of mmol.</p> <p>2.1.3 Stoichiometry of chemical reactions, concept of kg /mol, limiting reactant, theoretical and practical yield.</p> <p>2.1.4 Solubility and solubility equilibria, effect of presence of common ion in solution.</p> <p>2.1.5 Calculations of pH of acids, bases, acidic and basic buffers.</p> <p>2.1.6 Concept of formation constants, stability and instability constants, stepwise formation constants.</p> <p>2.1.7 Oxidation number, rules for assigning oxidation</p>	[15L]

		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 an oxidizing / reducing agent and its relationship with molarity).	
	3	<b>Optical Methods</b>	<b>[15 L]</b>
		<b>3.1 Infrared Absorption Spectroscopy [6 L]</b> 3.1.1 Instrumentation: Sources, Sample handling, Transducers, Dispersive, non-dispersive instrument. 3.1.2 Applications of IR [Mid IR, Near IR, Far IR]: Qualitative with emphasis on “Finger print” and Quantitative analysis. 3.1.3 Advantages and Limitations of IR.	
		<b>3.2 FT Technique [3 L]</b> 3.2.1 Introduction of Fourier Transform. 3.2.2 Laser as a source of radiation, sample containers. 3.2.3 Detectors, Fiber optics. 3.2.4 FTIR and its advantages.	
		<b>3.3 Molecular Ultraviolet and Visible Spectroscopy [6 L]</b> 3.3.1 Factors affecting molecular absorption: pH, temperature, solvent and effect of substituents, types of transitions [emphasis on charge transfer absorption]. 3.3.2 Applications of Ultraviolet and Visible spectroscopy: <ul style="list-style-type: none"> <li>i) On charge transfer absorption</li> <li>ii) Simultaneous spectroscopy</li> <li>iii) Derivative Spectroscopy</li> </ul> 3.3.3 Dual spectrometry – Introduction, Principle, Instrumentation and Applications.	
	4	<b>Instrumental methods-I</b>	<b>[15 L]</b>
		<b>4.1 Thermal Methods: [9 L]</b> 4.1.1 Introduction: Types of thermal methods, comparison between TGA and DTA. 4.1.2 Differential Scanning Calorimetry-Principle, comparison of DTA and DSC.	

		4.1.3 Instrumentation, Block diagram, Nature of DSC Curve, Factors affecting DSC Curves.	
		4.1.4 Applications - Heat of reaction, Safety screening, Polymers, liquid crystals, Drug analysis.	
		<b>4.2 Automation in chemical analysis: [6 L]</b>	
		4.2.1 Need for automation, Objectives of automation.	
		4.2.2 An overview of automated instruments.	
		4.2.3 Process control analysis, flow injection analysis, discrete automated system, automatic analysis based on multi-layered films, gas monitoring equipments.	
		4.2.4 Automatic titrators.	

## References

### Unit I

1. Modern Analytical Chemistry; David Harvey, McGraw-Hill, Higher Education,(2000)
2. Principles of Instrumental Analysis ; Skoog, Holler and Nieman, 5<sup>th</sup> Edition, Ch: 1
3. Fundamentals of Analytical Chemistry, Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, 9<sup>th</sup> Edition, 2004, Ch: 5.
4. Undergraduate Instrumental Analysis; J W Robinson, Marcel Dekker, 6<sup>th</sup> edition Ch:1.
5. ISO 9000 Quality Systems Handbook; David Hoyle. 4<sup>th</sup> edition (Chapter: 3 & 4) (Free download).
6. Quality in the Analytical Laboratory; Elizabeth Pichard, Wiley India, Ch: 5, Ch: 6 & Ch: 7.
7. Quality Management; Donna C S Summers, Prentice-Hall of India, Ch:3.
8. Quality in Totality: A Manager's Guide To TQM and ISO 9000, Parag Diwan, Deep & Deep Publications, 1st Edition, 2000.
9. Quality Control and Total Quality Management -; P.L. Jain-Tata McGraw-Hill (2006) Total Quality Management - Bester field - Pearson Education, Ch:5.
10. Industrial Hygiene and Chemical Safety, ; M H Fulekar, Ch:9, Ch:11 & Ch:15.
11. Safety and Hazards Management in Chemical Industries; M N Vyas, Atlantic Publisher, Ch:4, Ch:5 & Ch:19.
12. World Health Organization (2009) Handbook: Good Laboratory Practice (GLP)
13. OECD Principles of Good Laboratory Practice (as revised in 1997)". OECD Environmental Health and Safety Publications. OECD. 1. 1998
14. "A systematic approach for evaluating the quality of experimental toxicological and eco-toxicological data".; Klimisch, HJ; Andrae, M; Tillmann, U (1997). doi:10.1006/rtph.1996.1076. PMID 9056496.

### Unit II

1. 3000 solved problems in chemistry, Schaums Solved problem series, ; David E. Goldbers, Mc Graw Hill international Editions, Chapter 11,15,16,21,22

### Unit III

1. Principles of Instrumental Analysis, ; D. A. Skoog, F. J. Holler, T. A. Nieman, 5<sup>th</sup> Edition, Harcourt Asia Publisher. Chapter 6, 7,8, 13, 14, 16,17
2. Instrumental Methods of Analysis, H. H. Willard, L. L. Merritt, J. A. Dean, F. A. Settle, 6<sup>th</sup> Edition, CBS Publisher. Chapter 2.
3. Introduction to Instrumental Analysis, ; R. D. Braun , McGraw Hill Publisher. Chapter 5, 8, 12

4. Instrumental Methods of Chemical Analysis, ; G. W. Ewing, 5 th Edition, McGraw Hill Publisher, Chapter 3.
5. The effect of temperature on ultraviolet absorption spectra and its relation to hydrogen bonding,; M. Ito, J. Mol. Spectrosc. 4 (1960) 106-124.
6. The effect of temperature on the visible absorption band of iodine in several solvents; A. J. Somnessa, Spectrochim. Acta. Part A: Molecular Spectroscopy, 33 (1977) 525-528.
7. Infrared Spectroscopy- Materials Science, Engineering and Technology. Z. M. Khoshhesab (2012). Prof. Theophanides Theophile (Ed.). ISBN: 978-953- 51-0537- 4, InTech,(open access)

#### Unit IV

1. Introduction to instrumental methods of analysis; Robert D. Braun, Mc. Graw Hill (1987): Chapter 27,28
2. Thermal Analysis-theory and applications; R. T. Sane, Ghadge, Quest Publications
3. Instrumental methods of analysis; Willard, Merrit, Dean:7 th Edition, Chapter 25, 26
4. Instrumental Analysis, ; Skoog, Holler and Nieman, 5 th Edition, Chapter 31,33
5. Vogel's Quantitative Chemical Analysis,; 6 th Edition, Chapter 12
6. Analytical Chemistry - Open Learning: Thermal Methods; James W. Dodd, W. James and Kenneth H. Tonge

<b>PROGRAM(s): M.Sc.-I</b>				<b>SEMESTER: I</b>	
<b>Course: Mandatory Course Practicals</b>				<b>Course Code: PRCHEMAP 504</b>	
				<b>Course Title: - Chemistry Practical-I (Analytical Chemistry and organic Chemistry)</b>	
<b>Teaching Scheme</b>				<b>Evaluation Scheme</b>	
<b>Lectures (Hours per week)</b>	<b>Practical (Hours per week)</b>	<b>Tutorial (Hours per week)</b>	<b>Credit</b>	<b>Continuous Assessment (CA) (Marks- 25)</b>	<b>Semester End Examination (Marks- 25)</b>
				<b>50</b>	<b>50</b>
<b>NA</b>	<b>04</b>	<b>NA</b>	<b>02</b>		
<b>Learning Objectives:</b>					
1. To Gain knowledge of the advanced concepts in pH metry, quantum mechanics, potentiometry and conductometry experiments.					
2. To understand advance concept of thermodynamics and chemical kinetics in the chemical reactions.					
3. To develop scientific temper and research-based skills accomplish to encountered in the field of research.					

4. To gain knowledge and hands on experience in instrumental and non-instrumental analysis.
5. To introduce the concept of non-aqueous titrations.
6. To study technique of ion exchange and efficiency of the ion exchanger.
7. To develop scientific temper and research-based skills.

**Course Outcomes:**

1. To usage of subject fundamentals-principles with practical knowledge to design experiments, analyze and interpret data so as to reach to proper conclusions.
2. Learner will train the handling of equipments like potentiometer, conductivity meter, colorimeter and spectrophotometer.
3. Learner will develop scientific temper and research-based skills accomplish to encountered in the field of research.

The learner will be able to

4. handle and get familiar with SOP's of instruments like potentiometer, conductivity meter, colorimeter and spectrophotometer.
5. understand the concept of non-aqueous titrations and apply it in analysis of samples.
6. apply the theory of redox reactions to experimental systems.
7. separate the component of interest from the matrix.
8. develop scientific temperament and research-based skills accomplish to encountered in the field of research

## Chemistry Practical-I

**Course Code: PRCHEMAP 504**

	<b>Organic Chemistry</b>	<b>01</b>
	<p><b>One step preparation (1.0 g scale)</b></p> <ol style="list-style-type: none"> <li>1. Bromobenzene to p-nitrobromobenzene</li> <li>2. Anthracene to anthraquinone</li> <li>3. Benzoin to benzil</li> <li>4. Anthracene to Anthracene maleic anhydride adduct</li> <li>5. 2-Naphthol to BINOL</li> <li>6. p-Benzoquinone to 1,2,4-triacetoxybenzene</li> <li>7. Ethyl acetoacetate to 3-methyl-phenylpyrazol-5-one</li> <li>8. <i>o</i>-Phenylenediamine to 2-methylbenzimidazole</li> <li>9. <i>o</i>-Phenylenediamine to 2,3-diphenylquinoxaline</li> <li>10. Urea and benzil to 5,5-diphenylhydantoin</li> </ol> <p style="text-align: center;"><b>(Minimum 08 experiments are expected)</b></p>	
	<b>Analytical Chemistry</b>	<b>01</b>
	<p><b>Instrumental Experiments</b></p> <ol style="list-style-type: none"> <li>1. To determine percentage purity of sodium carbonate in</li> </ol>	

	<p>washing soda pH metrically.</p> <ol style="list-style-type: none"> <li>2. To determine amount of Ti(III) and Fe(II) in a mixture by titration with Ce(IV) potentiometrically.</li> <li>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.</li> <li>4. To determine the amount of nitrite, present in the given water sample colorimetrically.</li> </ol> <p><b>Non-Instrumental Experiments</b></p> <ol style="list-style-type: none"> <li>1.To carry out assay of the sodium chloride injection by Volhard's method.</li> <li>2.To determine (a) the ion exchange capacity (b) exchange efficiency of the given cation exchange resin.</li> <li>3.To determine amount of Cr(III) and Fe(II) individually in a mixture of the two by titration with EDTA.</li> <li>4.To determine number of nitro groups in the given compound using <math>TiCl_3</math>.</li> </ol>	
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**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.
4. Quantitative Inorganic Analysis including Elementary Instrumental Analysis by ; A. I. Vogels, 3rd Ed. ELBS (1964)
5. Vogel's textbook of quantitative chemical analysis, Mendham, Denny, Barnes, Thomas, Pearson education, Sixth Ed.
6. Standard methods of chemical analysis; F. J. Welcher, 1975
7. Standard methods of chemical analysis: Instrumental methods of Analysis ; F. J. Welcher , vol. 3, 1966
8. "Standard methods of Chemical Analysis"; W. W. Scott, Vol. I, Van Nostrand Company, Inc.,1939.
9. "Spectrophotometric Determination of Traces of Metals"; E.B.Sandell and H.Onishi, ,Part II,4th Ed. ,A Wiley Interscience Publication, New York,1978

**Elective-I**

**Course Title – Physical Chemistry -I**  
**Course Code: (CHEM 50211)**

<b>PROGRAM : M.Sc.-I</b>		<b>SEMESTER: I</b>			
<b>Course: Elective-I</b>		<b>Course Code: CHEM50211</b> <b>Course Title: - Physical Chemistry-I</b>			
<b>Teaching Scheme</b>					<b>Evaluation Scheme</b>
Lectures (Hours per week)	<b>Practical (Hours per week)</b>	<b>Tutorial (Hours per week)</b>	<b>Credit</b>	<b>Continuous Assessment (CA) (Marks-25)</b>	<b>Semester End Examination (Marks-25)</b>
02	NA	–	02		
<b>Learning Objectives:</b> <b>Physical Chemistry:</b> 1.To enable learners to have comprehensive knowledge and understanding of the advanced concepts in reaction kinetics, molecular dynamics and chemical thermodynamics. 2. To apply the basic knowledge of Physical chemistry to perform various tasks assigned to them at the workplace in industry and academia to meet the job requirements as per global standards. 3. Accomplish a solution to problems encountered in the field of research.					
<b>Course Outcomes:</b> 1. The learners will apply the advanced thermodynamics, Maxwell equation and its applications to ideal gases. 2. The learners evaluate the different theories of chemical kinetics and effect of temperature on reaction rates. 3. The learners will implement the applications of chemical thermodynamics to real gases, solutions, surfaces and their energetics. 4. The learners will understand the applications of operators and Schrodinger equation in the field of quantum Chemistry. 5. The learners will evaluate the resting membrane potential by using the concept of bio electrochemistry. 6. The learners will try to accomplish a solution to problems encountered in the field of research.					



Course Code: CHEM 50211	Unit	Course Title - Physical Chemistry – I Elective- I	Credits: 02 30L
	1	<b>Thermodynamics - I</b>	[15 L]
		<p><b>1.1</b> State function and exact differentials. Maxwell equations, Maxwell thermodynamic Relations; its 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]</p> <p><b>1.2</b> Third law 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.[7L]</p>	
	2	<p><b>Quantum Chemistry</b></p> <p>2.1. Classical Mechanics, failure of classical mechanics: Need for Quantum Mechanics.</p> <p>2.2 Particle waves and Schrödinger wave equation, wave functions, properties of wave functions, Normalization of wave functions, orthogonality of wave functions.</p> <p>2.3 Operators and their algebra, linear and Hermitian operators, operators for the dynamic variables of a system such as, position, linear momentum, angular</p>	[15L]

		<p>momentum, total energy, eigen functions, eigen values and eigen value equation, Schrödinger wave equation as the eigen value equation of the Hamiltonian operator, average value and the expectation value of a dynamic variable of the system, Postulates of Quantum Mechanics, Schrodinger's Time independent wave equation from Schrodinger's time dependent wave equation.</p> <p>2.4 Application of quantum mechanics to the following systems:</p> <ol style="list-style-type: none"> <li>a) Free particle, wave function and energy of a free particle.</li> <li>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.</li> <li>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]</li> </ol>	
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**[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> Edn., Oxford University Press, 2002.
2. K.J. Laidler and J.H. Meiser, *Physical Chemistry*, 2<sup>nd</sup> Ed., CBS Publishers and Distributors, New Delhi, 1999.
3. Robert J. Silby and Robert A. Alberty, *Physical Chemistry*, 3<sup>rd</sup> Edn., John Wiley and Sons (Asia) Pte. Ltd., 2002.
4. Ira R. Levine, *Physical Chemistry*, 5<sup>th</sup> Edn., Tata McGraw-Hill New Delhi, 2002.
5. G.W. Castellan, *Physical Chemistry*, 3<sup>rd</sup> Edn., Narosa Publishing House, New Delhi, 1983.
6. S. Glasstone, *Text Book of Physical Chemistry*, 2<sup>nd</sup> Edn., 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, *Quantum Chemistry*, 2<sup>nd</sup> Edn., New Age International Publishers, 2000.

## Elective - II

Course Title – Physical Chemistry II  
Course Code: (CHEM 50212)

PROGRAM: M.Sc.-I		SEMESTER: I			
Course: Elective-II		Course Code: CHEM50212 Course Title: - Physical Chemistry-II			
Teaching Scheme					Evaluation Scheme
Lectures (Hours per week)	Practical (Hours per week)	Tutorial (Hours per week)	Credit	Continuous Assessment (CA) (Marks-25)	Semester End Examination (Marks-25)
02	NA	–	02		
<b>Learning Objectives:</b> <b>Physical Chemistry:</b> 1. To enable learners to have comprehensive knowledge and understanding of the advanced concepts in reaction kinetics, molecular dynamics and chemical thermodynamics. 2. To apply the basic knowledge of Physical chemistry to perform various tasks assigned to them at the workplace in industry and academia to meet the job requirements as per global standards. 3. Accomplish a solution to problems encountered in the field of research.					
<b>Course Outcomes:</b> The learners will be able to:  1. The learners will apply the advanced thermodynamics, Maxwell equation and its applications to ideal gases. 2. The learners evaluate the different theories of chemical kinetics and effect of temperature on reaction rates. 3. The learners will implement the applications of chemical thermodynamics to real gases, solutions, surfaces and their energetics. 4. The learners will understand the applications of operators and Schrodinger equation in					

the field of quantum Chemistry.

5.The learners will evaluate the resting membrane potential by using the concept of bio electrochemistry.

6.The learners will try to accomplish a solution to problems encountered in the field of research.

<b>Course Code: CHEM 50212</b>	<b>Unit</b>	<b>Course Title - Physical Chemistry -II Elective- II</b>	<b>Credits: 02 30L</b>
	<b>1</b>	<b>Chemical Kinetics and Molecular Dynamics - I</b>	<b>[15 L]</b>
		<p>1.1 Composite Reactions:</p> <p>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.</p> <p>1.2 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.</p>	

		1.3 Reaction in Gas Phase Unimolecular Reactions: Lindeman-Hinshelwood theory, Rice-Ramsperger-Kassel (RRK) theory, Rice-Ramsperger-Kassel Marcus (RRKM) theory. [Ref. 2 and 5, 7, 8]	
	2	<b>Electrochemistry</b>	<b>[15L]</b>
		<p><b>2.1</b> Debye-Hückel theory of activity coefficient, Debye-Hückel limiting law and its extension to higher concentration (derivations are expected).</p> <p><b>2.2</b> 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.</p> <p><b>2.3</b> Batteries: Alkaline fuel cells, Phosphoric acid fuel cells, High temperature fuel cells [Solid – Oxide Fuel Cells (SOFC) and Molten Carbonate Fuel Cells</p> <p><b>2.4</b> 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: 4 and 6, 7, 8]</p>	

**[Note: Numerical and theoretical problems from each unit are expected**

### References:

1. S. Glasstone, *Thermodynamics for Chemists*, Affiliated East-West Press, New Delhi, 1964.
2. W.G. Davis, *Introduction to Chemical Thermodynamics – A Non – Calculus Approach*, Saunders, Philadelphia, 19772.
3. Peter A. Rock, *Chemical Thermodynamics*, University Science Books, Oxford University Press, 1983.
4. Ira N. Levine, *Quantum Chemistry*, 5<sup>th</sup> Edn., Pearson Education (Singapore) Pte. Ltd., Indian Branch, New Delhi, 2000.
5. Thomas Engel and Philip Reid, *Physical Chemistry*, 3<sup>rd</sup> Edn., Pearson Education Limited 2013.
6. D.N. Bajpai, *Advanced Physical Chemistry*, S. Chand 1<sup>st</sup> Edn., 1992.

7. *Bockris*, John O'M., *Reddy*, Amulya K.N., Gamboa-Aldeco, Maria E., Modern Electrochemistry, 2A, Plenum Publishers, 1998.
8. Physical Chemistry by Gurtu and Gurtu.
9. Dr. Harichandra A Parbat and Dr. Damodar V Prabhu, Essence of Chemical Kinetics, Sara Publication, First Edition, Sept. 2022.
10. A Text book of Physical Chemistry by K L Kapoor Vol 5 , 2<sup>nd</sup> Edn

**Elective Practical: Chemistry Practicals**  
**Course Code - CHEM 50211/ CHEM 50212**  
**Course Title – Inorganic Chemistry and Organic Chemistry**

<b>PROGRAM : M.Sc.-I</b>				<b>SEMESTER: I</b>
<b>Course: Elective Course Practicals</b>				<b>Course Code: CHEM 50211/ CHEM 50212</b>  <b>Course Title: - Inorganic Chemistry and Physical Chemistry</b>
<b>Teaching Scheme</b>				<b>Evaluation Scheme</b>
<b>Lectures (Hours per week)</b>	<b>Practical (Hours per week)</b>	<b>Credit</b>	<b>Continuous Assessment (CA) (Marks-25)</b>	<b>Semester End Examination (Marks- 25)</b>
----	<b>04</b>	<b>02</b>	<b>25</b>	<b>25</b>
<b>Learning Objectives:</b>				
<ol style="list-style-type: none"> <li>To develop practical skills such as decomposition of Alloys/Ores and carry out a Quantitative Analysis of the elements present in them.</li> <li>To learn the instrumental techniques to study properties of inorganic compound</li> <li>Planning of synthesis, effect of reaction parameters including stoichiometry, and safety aspects including MSDS should be learnt.</li> <li>Purify the product by crystallization. Formation and purity of the product should be checked by TLC</li> <li>Report mass and melting point of the purified product.</li> </ol>				
<b>Course Outcomes: Learners will be able to:</b>				
<ol style="list-style-type: none"> <li>To apply the knowledge of quantitative analysis for the determination of metals from ores/alloys.</li> <li>To have training of handling of instruments, and learning the techniques of instrumental analysis of various commercial inorganic compounds.</li> </ol>				

<b>Course Code: CHEM 50211/ CHEM 50212</b>	<b>Elective Practical: Chemistry Practicals</b>	<b>Credits 02</b>
	<b>Inorganic Chemistry</b>	<b>01</b>
	<p><b>Ores and Alloys</b>            1) Analysis of Devarda's alloy            2) Analysis of Cu – Ni alloy            3) Analysis of Limestone.            4) Analysis of Tin Solder alloy</p> <p><b>Instrumentation</b>            1) Estimation of Fe (III) solution using Ce (IV) ions Potentiometrically            2) Estimation of Copper using Iodometric method Potentiometrically            3) Estimation of Na<sub>2</sub>CO<sub>3</sub> in washing soda by pH metry            4) Estimation of Cl<sup>-</sup> ion in NaCl/KCl by Conductometry</p>	
<b>Course code- PRCHEMAP 504</b>	<b>Chemistry Practical-I</b>	<b>Credits:02</b>
	<b>Physical Chemistry</b>	<b>01</b>
	<p><b>Non – Instrumental:</b></p> <ol style="list-style-type: none"> <li>1. To determine the heat of solution (<math>\Delta H</math>) of a sparingly soluble acid (benzoic/salicylic acid) from solubility measurement at three different temperatures.</li> <li>2. To study the variation of calcium sulphate with ionic strength and hence determine the thermodynamic solubility product of CaSO<sub>4</sub> at room temperature.</li> <li>3. To investigate the reaction between acetone and iodine.</li> <li>4. Graph Plotting of mathematical functions –linear, exponential and trigonometry and identify whether functions are acceptable or non-acceptable?</li> </ol>	

	<b>Instrumental:</b>	
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1. To determine the mean ionic activity coefficient of an electrolyte by e.m.f. measurement.
2. To study the effect of substituent on the dissociation constant of acetic acid conductometrically.
3. To determine pKa values of phosphoric acid by potentiometric titration with sodium hydroxide using glass electrode.
4. To verify Ostwald's dilution law and to determine the dissociation constant of a weak mono-basic acid conductometrically.

**Reference:**

1. Advanced experiments in Inorganic Chemistry., G. N. Mukherjee., 1st 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: Dr Deepak Pant



## Research Methodology

<b>PROGRAM(s): M.Sc-I</b>		<b>SEMESTER: I</b>			
<b>Course code: CHEM506</b>		<b>Course Title: - Research Methodology</b>			
<b>Teaching Scheme</b>					<b>Evaluation Scheme</b>
<b>Lectures (Hours per week)</b>	<b>Practical (Hours per week)</b>	<b>Tutorial (Hours per week)</b>	<b>Credit</b>	<b>Continuous Assessment (CA) (Marks-50)</b>	<b>Semester End Examination (Marks- 50)</b>
<b>04</b>	–	–	<b>04</b>	<b>50</b>	<b>50</b>

### Learning Objectives:

1. To create awareness and understanding the terms like intellectual property, patents, copyright, industrial designs, trademarks, geographical indications etc.
2. To know trade secrets, IP infringement issues, economic value of intellectual property and study of various related international agreements.
3. To explore cheminformatics to facilitate molecular modeling and structure elucidations.
4. To apply the knowledge gained about various chemistry principles, techniques and tools in drug designing, target identification and validation, lead finding and optimization..

### Course Outcomes:

#### At the end of the Course,

1. To enable the student to be able to extract information from journals and digital resources.
2. Understanding tools to analyse the data, writing and presenting scientific papers.
3. Safe working procedure and ethical handling of chemicals.
4. Describe research, identification of research problems, and preparation of proposals.
5. Practice ethics in all the domains of research.
6. Analyze the results using mathematical and statistical tools.

<b>Course Code: - CHEM506</b>	<b>Unit</b>	<b>Course/ Unit Title: Research Methodology</b>	<b>04 Credits / 60 Lectures</b>
	<b>1</b>	<b>Literature Survey</b>	<b>15 L</b>
	<b>1.1</b>	Print:  Primary, Secondary and Tertiary sources. Journals: Journal abbreviations, abstracts, current titles,	<b>5 L</b>

		reviews, monographs, dictionaries, textbooks, current contents, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples.	
	<b>1.2</b>	Digital:  Web sources, E-journals, Journal access, TOC alerts, Hot articles, Citation Index, Impact factor, H-index, E-consortium, UGC infonet, E-books, Internet discussion groups and communities, Blogs, preprint servers, Search engines, Scirus, Google Scholar, ChemIndustry, Wiki-databases, ChemSpider, Science Direct, SciFinder, Scopus.	<b>5 L</b>
	<b>1.3</b>	Information Technology and Library Resources: The Internet and World wide web, Internet resources for Chemistry, finding and citing published information.	<b>5 L</b>
	<b>2</b>	<b>DATA ANALYSIS</b>	<b>15 L</b>
		The Investigative Approach: Making and recording Measurements, SI units and their use, Scientific methods and design of experiments. Analysis and Presentation of Data: Descriptive statistics, choosing and using statistical tests, Chemometrics, Analysis of Variance (ANOVA), Correlation and regression, curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, general polynomial fitting, linearizing transformations, exponential function fit, r and its abuse, basic aspects of multiple linear regression analysis.	
	<b>3</b>	<b>METHODS OF SCIENTIFIC RESEARCH AND WRITING SCIENTIFIC PAPERS</b>	<b>15 L</b>
		Reporting practical and project work, Writing literature surveys and reviews, organizing a poster display, giving an oral presentation. Writing Scientific Papers: Justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work, writing ethics, avoiding plagiarism.	
	<b>4</b>	<b>CHEMICAL SAFETY &amp; ETHICAL HANDLING OF CHEMICALS</b>	<b>15 L</b>
		Safe working procedure and protective environment,	

		<p>protective apparel, emergency procedure, first aid, laboratory ventilation, safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmospheric pressure, safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives, identification, verification and segregation of laboratory waste, disposal of chemicals in the sanitary sewer system, incineration and transportation of hazardous chemicals.</p>	
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**Reference books:-**

1. Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J., & Jones, A., (2011), Practical skills in Chemistry, 2 nd Ed., Prentice Hall, Harlow.
2. Hibbert, D. B. & Gooding, J. J. (2006) Data Analysis for Chemistry Oxford University Press.
3. Topping, J., (1984) Errors of Observation and their Treatment 4 th Ed., Chapman Hill, London.
4. Harris, D. C. (2007) Quantative Chemical Analysis 6 th Ed., Freeman Chapters 3-5
5. Levie, R. De. (2001) How to use Excel in Analytical Chemistry and in general scientific data analysis Cambridge Universty Press.
6. Chemical Safety matters – IUPAC-IPCS, (1992) Cambridge University Press.
7. OSU Safety manual 1.01

<b>PROGRAM(s): M.Sc.-I</b>		<b>SEMESTER: II</b>			
<b>Course:</b> Mandatory Course-I		<b>Course Code: CHEM507</b> <b>Course Title: - Inorganic Chemistry-II</b>			
<b>Teaching Scheme</b>					<b>Evaluation Scheme</b>
<b>Lectures (Hours per week)</b>	<b>Practical (Hours per week)</b>	<b>Tutorial (Hours per week)</b>	<b>Credit</b>	<b>Continuous Assessment (CA) (Marks- 50)</b>	<b>Semester End Examination (Marks- 50)</b>
<b>04</b>	<b>NA</b>	<b>-</b>	<b>04</b>	<b>50</b>	<b>50</b>

**Learning Objectives:**

**Inorganic Chemistry**

1. To have in depth understanding of mechanisms of inorganic reactions and methods used for determination of rate of reactions.
2. To gain knowledge of organometallic compounds with respect to synthesis structure and bonding.
3. To gain environmental consciousness through study of toxicity of metals and consequences of heavy metal pollution
4. To have extensive knowledge of significance of biological oxygen carriers and mechanism of enzyme catalytic reactions in biological systems.

**Course outcomes: -**

Learner will be able to:

- 1) elucidate on the rate, mechanism of inorganic reactions including substitution, redox and isomerization reactions and on the methods of determination of rate of reactions.
- 2) compare the stability of complexes elaborate different methods of preparation and analyze structure and bonding.
- 3) debate on toxicity of heavy metals, specific case studies and the effect of interaction of radiation with the environment
- 4) To infer role of biological oxygen carriers, copper containing enzymes and nitrogen fixing enzymes in biological systems

**Semester – II**

Course Code: - CHEM- 507	Unit	Course/ Unit Title: Inorganic Chemistry-II	04 Credits / 60 Lectures
	<b>1</b>	<p style="text-align: center;"><b>Inorganic Reaction Mechanism</b></p> <p><b>1.1</b> 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).</p> <p><b>1.2</b> Ligand substitution reactions of:</p> <p>a) Octahedral complexes without breaking of metal-ligand bond (Use of isotopic labelling method)</p> <p>b) Square planar complexes, trans-effect, its theories and applications. Mechanism and factors affecting these substitution reactions.</p> <p><b>1.3</b> Redox reactions: inner and outer sphere mechanisms, complimentary and non-complimentary reactions.</p> <p><b>1.4</b> Isomerization and racemization reactions</p>	[15 L]
	<b>2</b>	<p style="text-align: center;"><b>Organometallic Chemistry of Transition metals:</b></p> <p><b>2.1.</b> Eighteen electron rule and electron counting with examples, sixteen electron Square Planar complexes.</p> <p><b>2.2.</b> Preparation and properties of the following compounds</p> <p>(a) Alkyl and aryl derivatives of Pd and Pt complexes</p> <p>(b) Carbenes and carbynes of Cr, Mo and W</p> <p>(c) Alkene derivatives of Pd and Pt</p> <p>(d) Alkyne derivatives of Pd and Pt</p> <p>(e) Allyl derivatives of nickel</p> <p>(f) Sandwich compounds of Fe, Cr and Half Sandwich</p>	[15 L]

		<p>compounds of Cr, Mo.</p> <p><b>2.3</b> Structure and bonding on the basis of VBT and MOT in the following organometallic compounds:</p> <p>Zeise's salt, bis(triphenylphosphine)diphenylacetylene  platinum (0) [Pt(PPh<sub>3</sub>)<sub>2</sub>(HC≡CPh)<sub>2</sub>],  diallylnickel(diallylnickel(II), ferrocene and  bis(arene)chromium(0), tricarbonyl (<math>\eta^2</math>-butadiene) iron(0).</p>	
	3	<p style="text-align: center;"><b>Environmental Chemistry</b></p> <p><b>1.1.</b> Conception of Heavy Metals: Critical discussion on heavy metals</p> <p><b>1.2. Toxicity of metallic species:</b> a) Mercury, lead, cadmium, arsenic, copper and chromium, with respect to their sources, distribution, speciation, biochemical effects and toxicology, control and treatment.</p> <p>b) Itai-Itai disease for Cadmium toxicity,  c ) Arsenic Poisoning in the Indo-Bangladesh region.</p> <p><b>1.3. Interaction of radiation in context with the environment:</b> 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.</p>	[15 L]
	4	<p style="text-align: center;"><b>Bioinorganic Chemistry</b></p> <p>2.1. Biological oxygen carriers; haemoglobin, hemerythrene and hemocyanin- structure of metal active center and differences in mechanism of oxygen binding, Differences between haemoglobin and myoglobin: Cooperativity of oxygen binding in haemoglobin and Hill equation, pH dependence of oxygen affinity in haemoglobin and myoglobin and its implications.</p> <p>2.2. Activation of oxygen in biological system with examples</p>	[15 L]

	of mono-oxygenases 2.3. Copper containing enzymes- superoxide dismutase, 2.4. Nitrogen fixation-nitrogenase, hydrogenases 2.5. Metal ion transport and storage: Ionophores, transferrin, ferritin and metallothionins 2.6. Medicinal applications of cis-platin and related compounds	
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## References

### Unit- I

1. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Inorganic Chemistry, 5th Ed., Oxford University Press, 2010.
2. D. Banerjea, Coordination Chemistry, Tata McGraw Hill, 1993.
3. W. H. Malik, G. D./ Tuli and R. D. Madan, Selected Topics in Inorganic Chemistry, 8th Ed., S. Chand & Company ltd.
4. M. L. Tobe and J. Burgess, Inorganic Reaction Mechanism, Longman, 1999.
5. S. Asperger, Chemical kinetics and Inorganic Reaction Mechanism, 2nd Ed., Kluwer Academic/ Plenum Publishers, 2002
6. Gurdeep Raj, Advanced Inorganic Chemistry-Vol.II, 12th Edition, Goel publishing house,
7. B. R. Puri, L. R. Sharma and K. C. Kalia, Principles of Inorganic Chemistry, Milestone Publishers, 2013-2014.
8. F. Basalo and R. G. Pearson, Mechanism of Inorganic Reactions, 2nd Ed., Wiley, 1967.
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10. Robert B. Jordan, Reaction Mechanisms of Inorganic and Organometallic Systems, 3rd Ed., Oxford University Press 2008.

### Unit -II

1. D. Banerjea, Coordination chemistry. Tata McGraw Hill, New Delhi, 1993.
2. R.C Mehrotra and A.Singh, Organometallic Chemistry- A unified Approach, 2nd ed, New Age International Pvt Ltd, 2000.
3. R.H Crabtree, The Organometallic Chemistry of the Transition Metals, 5th edition, Wiley International Pvt, Ltd 2000.
4. B.Doughlas, D.H McDaniel and J.J Alexander. Concepts and Models of Inorganic Chemistry, 2nd edition, John Wiley and Sons. 1983.
5. Organometallic Chemistry by G.S Sodhi. Ane Books Pvt Ltd.

### Unit-III

1. Environmental Chemistry 5th edition, Colin Baird Michael Cann, W. H. Freeman and Company, New York, 2012.

2. Environmental Chemistry 7th edition, Stanley E. Manahan, CRC Press Publishers,
3. Environmental Contaminants, Daniel A. Vallero, ISBN: 0-12-710057-1, Elsevier Inc., 2004.
4. Environmental Science 13th edition, G. Tyler Miller Jr. and Scott E. Spoolman, ISBN-10: 0-495-56016-2, Brooks/Cole, Cengage Learning, 2010.
5. Fundamentals of Environmental and Toxicological Chemistry 4th edition, Stanley E. Manahan, ISBN: 978-1-4665-5317-0, CRC Press Taylor & Francis Group, 2013.
6. 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
7. Poisoning and Toxicology Handbook, Jerrold B. Leikin, Frank P. Paloucek, ISBN: 1-4200-4479-6, Informa Healthcare USA, Inc.
8. Casarett and Doull's Toxicology- The Basic Science of Poisons 6th edition, McGraw-Hill, 2001.

#### **Unit -IV**

1. R. W. Hay, *Bioinorganic Chemistry*, Ellis Harwood, England, 1984.
2. I. Bertini, H.B.Gray, S. J. Lippard and J.S. Valentine, *Bioinorganic Chemistry*, First South Indian Edition, Viva Books, New Delhi, 1998.
3. J. A. Cowan, *Inorganic Biochemistry-An introduction*, VCH Publication, 1993.
4. S. J. Lippard and J. M. Berg, *Principles of Bioinorganic Chemistry*, University Science Publications, Mill Valley, Caligronic, 1994.
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
9. J. R. Frausto da Silva and R. J. P. Williams *The Biological Chemistry of the Elements*, Clarendon Press, Oxford, 1991.
10. JM. D. Yudkin and R. E. Offord *A Guidebook to Biochemistry*, Cambridge University Press, 1980



<b>PROGRAM: M.Sc.-I</b>		<b>SEMESTER: II</b>			
Course: Mandatory Course -II		<b>Course Code: CHEM 509</b> <b>Course title: Organic Chemistry-II</b>			
<b>Teaching Scheme</b>					<b>Evaluation Scheme</b>
<b>Lectures</b>  <b>(Hours per week)</b>	<b>Practical</b>  <b>(Hours per week)</b>	<b>Tutorial</b> <b>I</b> <b>(Hours per week)</b>	<b>Credit</b>	<b>Continuous Assessment (CA)</b> <b>(Marks- 50)</b>	<b>Semester End Examination</b> <b>(Marks- 50)</b>
<b>04</b>	<b>NA</b>	<b>–</b>	<b>04</b>	<b>50</b>	<b>50</b>
<b>Learning Objectives:</b>					
<p>1.To enable learners to have comprehensive knowledge and understanding of the advanced concepts in reaction Mechanism, molecular orbital theory, different rearrangement reactions and spectroscopic techniques.</p> <p>2. To apply the basic knowledge of Organic chemistry to perform various tasks assigned to them at the workplace in industry and academia to meet the job requirements as per global standards.</p> <p>3. Accomplish a solution to problems encountered in the field of research.</p>					
<b>Course Outcomes:</b>					
<p>After completing the course students will be able to:</p> <ol style="list-style-type: none"> <li>1) Recognize the type of mechanism &amp; intermediates involved in the given organic reaction and to prove mechanism for the reaction.</li> <li>2) Identify the ways to modify aliphatic and aromatic compounds via Nucleophilic substitution reactions.</li> <li>3) Predict the mechanism and stereochemistry of important organic reactions.</li> <li>4) Understand and write the mechanism of rearrangement reactions with stereochemistry and its applications.</li> <li>5) Understand the HOMO-LUMO concept and its significance in organic chemistry.</li> <li>6) Understand the basic principle and concepts in UV and IR spectroscopy</li> <li>7) Understand the basic concepts of <math>^1\text{H}</math>, <math>^{13}\text{C}</math> NMR, and mass spectroscopy.</li> <li>8) Understand how <math>^1\text{H}</math>, <math>^{13}\text{C}</math> NMR and Mass spectroscopy are important for the structure determination of organic compounds.</li> </ol>					

Course Code:- CHEM 509	Unit	Course/ Unit Title: Organic Chemistry -II	04 Credits / 60 Lectures
	1	<p><b>1.1. Alkylation of Nucleophilic Carbon Intermediates:</b></p> <p>1.1.1. Generation of carbanion, kinetic and thermodynamic enolate formation, Regioselectivity in enolate formation, alkylation of enolates.</p> <p>1.1.2. Generation and alkylation of dianion, medium effects in the alkylation of enolates, oxygen versus carbon as the site of alkylation.</p> <p>1.1.3. Alkylation of aldehydes, ketones, esters, amides and nitriles.</p> <p>1.1.4. Nitrogen analogs of enols and enolates- Enamines and Imines anions, alkylation of enamines and imines.</p> <p>1.1.5. Alkylation of carbon nucleophiles by conjugate addition (Michael reaction).</p>	(7 L)
		<p><b>1.2. Reaction of carbon nucleophiles with carbonyl groups:</b></p> <p>1.2.1. Mechanism of Acid and base catalyzed Aldol condensation, Mixed Aldol condensation with aromatic aldehydes, Regio chemistry in mixed reactions of aliphatic aldehydes and ketones, intramolecular Aldol reaction and Robinson annulation.</p> <p>1.2.2. Addition reactions with amines and iminium ions; Mannich reaction.</p> <p>1.2.3. Amine catalyzed condensation reaction: Knoevenagel reaction.</p> <p>1.2.4. Acylation of carbanions</p>	(8 L)
	2	<p><b>2.1 Introduction to Molecular Orbital Theory for Organic Chemistry:</b></p> <p><b>2.1.1. Molecular orbitals:</b> Formation of <math>\sigma</math>- and <math>\pi</math>-MOs by using LCAO method. Formation of <math>\pi</math> MOs of ethylene, butadiene, 1, 3, 5-hexatriene, allyl cation, anion and radical. Concept of nodal planes and energies of <math>\pi</math>-MOs</p> <p><b>2.1.2. Introduction to FMOs:</b> 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 (<math>\pi</math> and <math>\pi^*</math> orbitals) of formaldehyde. A brief description of MOs of nucleophiles and electrophiles. Concept of 'donor-</p>	(7L)

		<p>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.</p> <p><b>2.1.3.</b> Application of FMO concepts in (a) <math>S_N^2</math> reaction, (b) Lewis acid base adducts (<math>BF_3-NH_3</math> complex), (c) ethylene dimerization to Cyclobutane, (d) Diels-Alder cycloaddition, (e) regioselective reaction of allyl cation with allyl anion (f) addition of hydride to formaldehyde.</p>	
		<p><b>2.2. Applications of UV and IR spectroscopy:</b></p> <p><b>2.2.1. Ultraviolet spectroscopy:</b> 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).</p> <p><b>2.2.2. Infrared spectroscopy:</b> 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.</p>	(8L)
	3	<p><b>Reactions and Rearrangements:</b></p> <p>Mechanisms, stereochemistry (if applicable) and applications of the following:</p> <p><b>3.1. Reactions:</b> Baylis-Hillman reaction, McMurry Coupling, Corey-Fuchs reaction, Nef reaction,</p>	(15L)

		<p>Passerini reaction.</p> <p><b>3.2. Concerted rearrangements:</b> Hofmann, Curtius, Lossen, Schmidt, Wolff, Boulton-Katritzky.</p> <p><b>3.3. Cationic rearrangements:</b> Tiffeneau-Demjanov, Pummerer, Dienone-phenol, Rupe, Wagner-Meerwein.</p> <p><b>3.4. Anionic rearrangements:</b> Brook, Neber, Von Richter, Wittig, Gabriel-Colman, Baker-Venkataraman.</p>	
	<b>4</b>	<p><b><sup>1</sup>H and <sup>13</sup>C NMR spectroscopy and Mass spectrometry</b></p> <p><b>4.1. Proton magnetic resonance spectroscopy:</b> Principle, Chemical shift, Factors affecting on 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, Karplus equation, long range coupling (allylic and aromatic).</p> <p><b>4.2. <sup>13</sup>C NMR spectroscopy:</b> 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.</p> <p><b>4.3. Mass spectrometry:</b> Basic Principle, 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.</p> <p><b>4.4.</b> Structure determination involving individual or combined use of the above spectral techniques.</p>	<b>(15L)</b>

## References:

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2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Part A, page no. 713-769, and B, Plenum Press.
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.
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11. Mechanism in Organic Chemistry, Peter Sykes, 6<sup>th</sup>
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. Parashar, Alpha Science International, 2011.
20. Name Reactions, Jie Jack Li, Springer
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22. Reactions, Rearrangements and Reagents by S.N. Sanyal.
23. Name Reactions, Jie Jack Li, Springer.
24. Name reactions and Reagents in Organic Synthesis, Bradford P. Mundy, M.G. Ellerd and F.G. Favaloro, John Wiley & Sons.
25. Organic reactions and their Mechanisms, P.S. Kalsi, New Age International Publishers.
26. Elementary Organic Spectroscopy By- Y R Sharma, (S. Chand Publications)

<b>PROGRAM(s): M.Sc.-I</b>				<b>SEMESTER: II</b>
<b>Course : Mandatory course - III</b>				<b>Course Code: (CHEM 510)</b> <b>Course Title:-Analytical Chemistry-II</b>
<b>Teaching Scheme</b>				<b>Evaluation Scheme</b>
<b>Lectures (Hours per week)</b>	<b>Practical (Hours per week)</b>	<b>Credit</b>	<b>Continuous Assessment (CA) (Marks-50)</b>	<b>Semester End Examination (Marks- 50)</b>
<b>04</b>	<b>NA</b>	<b>04</b>	<b>50</b>	<b>50</b>
<b>Course Objectives:</b>				
<ol style="list-style-type: none"> <li>1. To gain knowledge of the chromatography techniques and its applications.</li> <li>2. To understand application of X-ray spectroscopy for qualitative and quantitative analysis.</li> <li>3. To introduce radio analytical techniques.</li> <li>4. To apply the surface analytical techniques for system.</li> <li>5. To study advantages and applications of electroanalytical methods.</li> </ol>				
<b>Course outcomes: -</b>				
After completion of this Course, the learner will be				
<ol style="list-style-type: none"> <li>1. able to compare the advantages/disadvantages of SEM, STM and TEM.</li> <li>2. able to develop different techniques to separate the components of mixture.</li> <li>3. conversant with basic principles and theories of mass spectrometry.</li> <li>4. able to apply the electroanalytical methods to sample under consideration.</li> <li>5. able to elaborate on electrogravimetry and coulometry techniques.</li> </ol>				

<b>Course Code:- CHEM 510</b>	<b>Unit</b>	<b>Course/ Unit Title: Analytical Chemistry-II</b>	<b>04 Credits / 60 Lectures</b>
	<b>1</b>	<b>Chromatography</b>	<b>15L</b>

	<b>1.1</b>	<p><b>Basic concepts and theories of chromatography: [5 L]</b></p> <p><b>1.1.1</b> Introduction and Classification of chromatographic methods.</p> <p><b>1.1.2</b> Concept of plate and rate theories in chromatography, efficiency, resolution, selectivity and separation capability.</p> <p><b>1.1.3</b> Van Deemter equation and broadening of chromatographic peaks. Optimization of chromatographic conditions.</p>	
	<b>1.2</b>	<p><b>Gas Chromatography: [5 L]</b></p> <p><b>1.2.1</b> Instrumentation –sample injection systems (split/split less), column types (solid/ liquid stationary phases), column switching techniques, temperature programming.</p> <p><b>1.2.2</b> Requirements of an ideal detector and types of detectors in GLC and GSC.</p> <p><b>1.2.3</b> Applications -Qualitative and quantitative analysis.</p>	
	<b>1.3</b>	<p><b>High Performance Liquid Chromatography (HPLC):[5 L]</b></p> <p><b>1.3.1</b> Normal phase and reversed phase with special reference to types of commercially available columns (Use of C8 and C18 columns).</p> <p><b>1.3.2</b> Diode array type and fluorescence detector.</p> <p><b>1.3.3</b> Applications of HPLC.</p>	
	<b>2</b>	<b>Instrumental methods – II</b>	<b>15L</b>
		<p><b>2.1 X-ray spectroscopy: [6 L]</b> Principle, instrumentation, applications, advantages and limitations of</p> <p><b>2.1.1</b> X-ray absorption spectroscopy. (XAS)</p> <p><b>2.1.2</b> X-ray fluorescence spectroscopy (XRF)</p> <p><b>2.1.3</b> X-ray diffraction spectroscopy. (XRD)</p>	
		<p><b>2.2 Mass spectrometry: [6 L]</b></p> <p><b>2.2.1</b> Instrumentation -</p> <p>i) on sources - electron impact, field ionization, field absorption, chemical ionization and fast atom bombardment sources.</p> <p>ii) Mass analyzers: Quadrupole, time of flight and ion trap.</p> <p><b>2.2.2</b> Applications</p>	
		<p><b>2.3 Radio analytical Methods – [3 L]</b></p> <p><b>2.3.1</b> Neutron Activation Analysis (NAA)- Introduction,</p>	

		Principle, Theory and Applications. <b>2.3.2 Advantages and Limitations of NAA.</b>	
	<b>3</b>	<b>Instrumental methods – III</b>	<b>15L</b>
	3.1	<b>Surface Analytical Techniques – [9 L]</b> Principle, Instrumentation and Applications of: <b>3.1.1 Scanning Electron Microscopy (SEM)</b> <b>3.1.2 Scanning Tunneling Microscopy (STM)</b> <b>3.1.3 Transmission Electron Microscopy (TEM)</b>	
	3.2	<b>Atomic Spectroscopy [6 L]</b> <b>3.2.1 Atomic Spectroscopy based on plasma sources – Introduction, Principle, Instrumentation and Applications.</b> <b>3.2.2 Advantages and Limitations of AAS</b>	
	<b>4</b>	<b>Electroanalytical Methods</b>	<b>15L</b>
	4.1	<b>Ion selective potentiometry and Polarography: [10L]</b> <b>4.1.1</b> Ion selective electrodes: Applications of - solid state, precipitate, liquid –liquid, enzyme, gas sensing, bio-catalytic membrane and enzyme-based biosensors electrodes. <b>4.1.2</b> Polarography: Ilkovic equation, Cottrell equation, effect of complex formation on the polarographic waves.	
	4.2	<b>Electrogravimetry: [2 L]</b> <b>4.2.1</b> Introduction, Principle and Instrumentation. <b>4.2.2</b> Factors affecting the nature of the deposit. <b>4.2.3</b> Applications.	
	4.3	<b>Coulometry: [3 L]</b> <b>4.3.1</b> Introduction, Principle and Instrumentation. <b>4.3.2</b> Coulometry at controlled potential and controlled current.	



## References:

### Unit- I

1. Instrumental Analysis, Skoog, Holler and Crouch, 7<sup>th</sup> edition
2. HPLC Practical and Industrial Applications; E.B.Sandell and H.Onishi 2<sup>nd</sup> Ed., CRC Press

### Unit -II

1. Essentials of Nuclear Chemistry; H J Arnikaar, New Age Publishers (2005)
2. Fundamentals of Radiochemistry; D. D. Sood A. V. R. Reddy and N. Ramamoorthy, , IANCAS 4<sup>th</sup> edition, 2010
3. Principles of Instrumental Analysis - Skoog, Holler and Nieman, 5<sup>th</sup> Edition, Ch: 12, 20

### Unit- III

1. Instrumental Analysis; Douglas A. Skoog - F. James Holler - Crouch, Publisher: Cengage; Edition, (2003), ISBN-10: 8131505421, ISBN-13: 978-8131505427
2. Physical Principles of Electron Microscopy, An Introduction to TEM, SEM, and AEM  
; Ray F. Egerton, ISBN: 978-0- 387-25800- 3 (Print) 978-0- 387-26016- 7 (Online)
3. Modern techniques of surface science; D.P. Woodruff and T.A. Delchar, Cambridge Univ. Press, 1994.
4. Introduction to Scanning Tunneling Microscopy ; C. J. Chen, Oxford University Press, New York, 1993.
5. Transmission Electron Microscopy: A text book for Material Science; David B Williams and C., Barry Carter, Springer, 2009
6. Modern Spectroscopy,; J.M. Hollas, , John Wiley, New York, 3rd Edition (1996),
7. Principles of Instrumental Analysis; Skoog, Holler, Nieman, Harcourt College Publishers, 5th ed., 1998.
8. Instrumental Analysis; Douglas A. Skoog - F. James Holler - Crouch, Publisher: Cengage; Edition (2003), ISBN10: 8131505421, ISBN-13: 978-8131505427

### Unit -IV

1. Principles of Instrumental Analysis – ; Skoog, Holler, Nieman, Harcourt College Publishers, 5<sup>th</sup> Edition, 1998. Chapters - 23, 24, 25.
2. Analytical Chemistry Principles – ; John H Kennedy, Saunders College Publishing, 2nd edition, (1990).
3. Modern Analytical Chemistry; David Harvey; McGraw Hill Higher education publishers, (2000).
4. Vogel's Text book of quantitative chemical analysis; Pearson Education Limited, 6th edition, (2007).
5. Electrochemical Methods Fundamentals and Applications; Allen J Bard and Larry R Faulkner, John Wiley and Sons, (1980).
6. Instrumental Methods of Analysis; Willard, Merrit, Dean and Settle, CBS publishers, 7th edition

## Semester II

### Chemistry Practical-II Analytical Chemistry and Physical Chemistry

<b>PROGRAM(s): M.Sc.-I</b>				<b>SEMESTER: II</b>
<b>Course : Mandatory Course Chemistry Practicals II</b>				<b>Course Code:</b> PRCHEMAP 511  <b>Course Title:</b> - Analytical Chemistry and Organic Chemistry
<b>Teaching Scheme</b>				<b>Evaluation Scheme</b>
<b>Lectures (Hours per week)</b>	<b>Practical (Hours per week)</b>	<b>Credit</b>	<b>Continuous Assessment (CA) (Marks- 25)</b>	<b>Semester End Examination (Marks- 25)</b>
NA	04	02		
<b>Learning Objectives:</b> 1.To gain knowledge of the advanced concepts in pH metry, quantum mechanics, potentiometry and conductometry experiments. 2.To develop scientific temper and research-based skills accomplish to encountered in the field of research. 3.To gain knowledge and hands on experience in instrumental and non-instrumental analysis. 4.To introduce the concept of simultaneous determination in spectrophotometry. 5. To study technique of ion exchange and breakthrough capacity. 6. To develop scientific temper and research-based skills.				
<b>Course Outcomes: -</b> 1.To use the concept of quantum chemistry to interpret the shape and information about the orbitals like 1s, 2pz and 3dz <sup>2</sup> . 2. To apply the subject fundamentals-principles with practical knowledge to design experiments, analyze and interpret data so as to reach to proper conclusions 3. Learner will train to handle the sophisticated instrument like digital potentiometer, conductivity meter, spectrophotometer. After completion of this Course, the learner will be able to 1. handle and get familiar with SOP's of instruments like potentiometer, conductivity meter, colorimeter and spectrophotometer. 2. understand the concept of complexometric titrations and factors enhancing selectivity of EDTA as a titrant. 3. apply the theory of FES to fertilizers analysis. 4. develop scientific temperament and research-based skills accomplish to encountered in the field of research				

<b>Course code:- PRCHEMA P 511</b>	<b>Chemistry Practical-II</b>	<b>Credits 02</b>
	<p style="text-align: center;"><b>Organic Chemistry</b></p> <p><b>Separation of Binary mixture using micro-scale technique</b>  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.  <b>(Minimum two mixtures from each type and a total of eight mixtures are expected.)</b></p>	<b>01</b>
	<b>Analytical Chemistry</b>	<b>01 Credit</b>
	<p><b>Instrumental Experiments</b></p> <ol style="list-style-type: none"> <li>1. To determine the amount of Fe(II) and Fe(III) in a mixture using 1,10-phenanthroline spectrophotometrically.</li> <li>2. Simultaneous determination of Cr(VI) and Mn(VII) in a mixture spectrophotometrically.</li> <li>3. 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>.</li> <li>4. To determine amount of potassium in the given sample of fertilizers using flame photometer by standard addition method.</li> </ol> <p><b>Non-Instrumental Experiments</b></p> <ol style="list-style-type: none"> <li>1. To determine the lead and tin content of a solder alloy by titration with EDTA.</li> <li>2. To determine amount of Cu(II) present in the given solution containing a mixture of Cu(II) and Fe(II).</li> <li>3. To determine the break through capacity of a cation exchange resin.</li> <li>4. Estimation of a mixture of Hydrochloric acid and boric</li> </ol>	

**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.
4. Quantitative Inorganic Analysis including Elementary Instrumental Analysis by ; A. I. Vogels, 3rd Ed. ELBS (1964)
5. Vogel's textbook of quantitative chemical analysis, Mendham, Denny, Barnes, Thomas, Pearson education, Sixth Ed.
6. Standard methods of chemical analysis; F. J. Welcher, 1975
7. Standard methods of chemical analysis: Instrumental methods of Analysis ; F. J. Welcher , vol. 3, 1966
8. "Standard methods of Chemical Analysis"; W. W. Scott, Vol. I, Van Nostrand Company, Inc.,1939.
9. "Spectrophotometric Determination of Traces of Metals"; E.B.Sandell and H.Onishi, ,Part II,4th Ed. ,A Wiley Interscience Publication, New York,1978

**Course Code: CHEM 50811**  
**Course Title: Physical Chemistry-III**

<b>PROGRAM(s): M.Sc.-I</b>		<b>SEMESTER: II</b>			
<b>Course: Elective -I</b>		<b>Course Code: CHEM50811</b> <b>Course Title: - Physical Chemistry-III</b>			
<b>Teaching Scheme</b>					<b>Evaluation Scheme</b>
<b>Lectures (Hours per week)</b>	<b>Practical (Hours per week)</b>	<b>Tutorial (Hours per week)</b>	<b>Credit</b>	<b>Continuous Assessment (CA) (Marks- 25)</b>	<b>Semester End Examination (Marks- 25)</b>
<b>02</b>	<b>NA</b>	<b>–</b>	<b>02</b>		
<b>Learning Objectives:</b>					
<ol style="list-style-type: none"> <li>To gain knowledge of the advanced concepts in quantum mechanics, applications of HMO theory, chemical kinetics and molecular dynamics.</li> <li>To understand the advanced concepts in chemical thermodynamics and photochemistry.</li> <li>To develop the skill to solve the problems encountered in the field of quantum and electrochemistry.</li> </ol>					
<b>Course Outcomes:</b>					
<ol style="list-style-type: none"> <li>To learn the concept of quantum chemistry and able to solve problems related to 1D box, 2D box, 3D box and to explain the role of operators in quantum chemistry.</li> <li>To understand the use of Schrodinger wave equation in one and two electron systems along with applications of HMO.</li> <li>To develop the skill to solve the problems based on chemical thermodynamics, molecular dynamics and quantum Chemistry.</li> <li>To apply the concept of Jablonski mechanism in photochemical reactions.</li> <li>Learners will get knowledge of advanced chemical kinetics and molecular dynamics.</li> </ol>					

<b>Course Code:- CHEM 50811</b>	<b>Unit</b>	<b>Course/ Unit Title: Physical Chemistry-III</b>	<b>02 Credits / 30 Lectures</b>
	<b>1</b>	<b>Chemical Thermodynamics II</b>	<b>[15 L]</b>
	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	<b>Real solutions:</b> Chemical potential in non-ideal solutions excess functions of non-ideal solutions calculation of partial molar volume and partial molar enthalpy, Gibbs Duhem Margules equation.	
	1.3	<b>Thermodynamics of surfaces,</b> Pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, BET isotherm (derivations expected).	
	1.4	<b>Bioenergetics:</b> standard free energy change in biochemical reactions, exergonic, endergonic. Hydrolysis of ATP, synthesis of ATP from ADP. [Ref 2 and 1,10,11,12]	
	<b>2</b>	<b>Quantum Chemistry II</b>	<b>[15 L]</b>
	2.1	Rigid rotor, spherical coordinates Schrödinger wave equation in spherical coordinates, separation of the variables, the phi equation, wavefunction, 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 Radial (R), Zenith (theta) and Azimuthal (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.	
	2.3.	Application of the Schrödinger equation to two electron system, 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, cyclobutadiene and benzene. <i>(Derivation expected)</i>	

		[Ref 7, 8 and 9]	
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## References

1. Peter Atkins and Julio de Paula, *Atkins's Physical Chemistry*, 7<sup>th</sup> Edn., Oxford University Press, 2002.
2. K.J. Laidler and J.H. Meiser, *Physical Chemistry*, 2<sup>nd</sup> Ed., CBS Publishers and Distributors, New Delhi, 1999.
3. Robert J. Silby and Robert A. Alberty, *Physical Chemistry*, 3<sup>rd</sup> Edn., John Wiley and Sons (Asia) Pte. Ltd., 2002.
4. Ira R. Levine, *Physical Chemistry*, 5<sup>th</sup> Edn., Tata McGraw-Hill New Delhi, 2002.
5. G.W. Castellan, *Physical Chemistry*, 3<sup>rd</sup> Edn., Narosa Publishing House, New Delhi, 1983.
6. S. Glasstone, *Text Book of Physical Chemistry*, 2<sup>nd</sup> Edn., McMillan and Co. Ltd., London, 1962.
7. Principles of Chemical Kinetics, 2<sup>nd</sup> Ed., James E. House, ELSEVIER, 2007.
8. B.K. Sen, *Quantum Chemistry including Spectroscopy*, Kalyani Publishers, 2003.
9. A.K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw – Hill, 1994.
10. R.K. Prasad, *Quantum Chemistry*, 2<sup>nd</sup> Edn., New Age International Publishers, 2000.
11. S. Glasstone, *Thermodynamics for Chemists*, Affiliated East-West Press, New Delhi, 1964.
12. W.G. Davis, *Introduction to Chemical Thermodynamics – A Non – Calculus Approach*, Saunders, Philadelphia, 19772.
13. Peter A. Rock, *Chemical Thermodynamics*, University Science Books, Oxford University Press, 1983.
14. Ira N. Levine, *Quantum Chemistry*, 5<sup>th</sup> Edn., Pearson Education (Singapore) Pte. Ltd., Indian Branch, New Delhi, 2000.

**Course Code: CHEM 50812**  
**Course Title: Physical Chemistry-IV**

<b>PROGRAM(s): M.Sc.-I</b>		<b>SEMESTER: II</b>			
Course: Elective -II		Course Code: CHEM50812 Course Title: - Physical Chemistry-IV			
Teaching Scheme					Evaluation Scheme
Lectures (Hours per week)	Practical (Hours per week)	Tutorial (Hours per week)	Credit	Continuous Assessment (CA) (Marks- 25)	Semester End Examination (Marks- 25)

02	NA	-	02		
<b>Learning Objectives:</b> <b>Physical Chemistry</b> 1To gain knowledge of the advanced concepts in quantum mechanics, applications of HMO theory, chemical kinetics and molecular dynamics. 2To understand the advanced concepts in chemical thermodynamics and photochemistry. 3To develop the skill to solve the problems encountered in the field of quantum and electrochemistry.					
<b>Course Outcomes:</b> The student will be able to: 1.To understand the use of Schrodinger wave equation in one and two electron systems along with applications of HMO. 2.To develop the skill to solve the problems based on chemical thermodynamics, molecular dynamics and quantum Chemistry. 3.To apply the concept of Jablonski mechanism in photochemical reactions. 5Learners will get knowledge of advanced chemical kinetics and molecular dynamics.					

Course Code:- CHEM 50812	Unit	Course/ Unit Title: Physical Chemistry-IV	02 Credits / 30 Lectures
	1	<b>Chemical Kinetics and Molecular Dynamics-II</b>	[15 L]
	1.1.	<b>Elementary Reactions in Solution:</b> - Solvent Effects on reaction rates, Reactions between ions- influence of solvent Dielectric constant, influence of ionic strength, Linear free energy relationships Enzyme action.	
	1.2.	<b>Kinetics of reactions catalyzed by enzymes</b> -Michaelis-Menten analysis, Lineweaver-Burk and Eadie Analyses.	
	1.3.	<b>Inhibition of Enzyme action:</b> Competitive, Noncompetitive and Uncompetitive Inhibition. Effect of pH, Enzyme activation by metal ions, Regulatory enzymes.	
	1.4.	<b>Kinetics of reactions in the Solid State:</b> - Factors affecting reactions in solids <b>Rate laws for reactions in solid:</b> 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, 22)	



	<b>2</b>	<b>Photochemistry</b>	<b>[15 L]</b>
	<b>2.1</b>	Absorption of light, laws of photochemistry, electronic structure of molecules, molecular orbital, electronically excited singlet states, designation based on multiplicity rule, construction of Jablonski diagram, electronic transition, Frank Condon principle, selection rules, intensity of absorption bands, nature of electronic spectra and primary process, photo-dissociation, pre-dissociation.	
	<b>2.2</b>	Photo physical phenomena: physical pathways of excited molecular system (radiative and non-radiative), prompt fluorescence, delayed fluorescence, and phosphorescence, fluorescence quenching: concentration quenching, collisional quenching, quenching by excimer and exciplex emission, fluorescence resonance energy transfer between photo-excited donor and acceptor systems.	
	<b>2.3.</b>	Stern-Volmer relation, critical energy transfer distances, energy transfer efficiency, examples and applications in chemical analysis. Photochemical reactions, photo-oxidation, photoreduction, photo-dimerization, photoisomerization and photosensitized reactions. Photochemistry of environment: Greenhouse effect.	

### References:

1. Thomas Engel and Philip Reid, Physical Chemistry, 3<sup>rd</sup> Edn., Pearson Education Limited 2013.
2. D.N. Bajpai, Advanced Physical Chemistry, S. Chand 1<sup>st</sup> Edn., 1992.
3. C. H. DePuy, O. L. Chapman, Molecular reactions and photo Chemistry, Prenticehall of India PVT.LTD.1988.
4. K. K. Rohatgi-Mukherjee. Fundamentals of Photochemistry. Reprint 2002. New Age International Publisher, 1978.
5. Principles of physical Chemistry , Marrown and Prutton 5<sup>th</sup> edition
6. Essentials of Physical Chemistry , Arun Bahl, B. S Bahl, G. D.Tulli , S Chand and Co. Ltd , 2012 Edition.
7. Introduction of Solids L.V Azaroff , Tata McGraw Hill .
8. Dr. Harichandra A Parbat and Dr. Damodar V Prabhu, Essence of Chemical Kinetics, Sara Publication, First Edition, Sept. 2022.
9. A Text book of physical Chemistry ; Applications of thermodynamics vol III, Mac Millan Publishers India Ltd, 2011
10. New directions in solid state Chemistry, C.N.R. Rao and J Gopalkrishnan , Cambridge University Press.

## Chemistry Practicals (Inorganic Chemistry and Organic Chemistry)

Course Code: CHEM 50811/CHEM 50812

<b>PROGRAM(s): M.Sc.-I</b>				<b>SEMESTER: II</b>
<b>Course : Elective Course Chemistry Practicals</b>				<b>Course Code:</b> CHEM 50811/CHEM 50812 <b>Course Title: - Inorganic Chemistry and Physical Chemistry</b>
<b>Teaching Scheme</b>				<b>Evaluation Scheme</b>
<b>Lectures (Hours per week)</b>	<b>Practical (Hours per week)</b>	<b>Credit</b>	<b>Continuous Assessment (CA) (Marks- 25)</b>	<b>Semester End Examination (Marks- 25)</b>
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### Learning Objectives:

1. To understand the application of theoretical concept of metal ligand coordination by synthesizing inorganic complexes
2. To learn the established instrumental techniques in order to study properties of inorganic compounds.
3. To learn Organic mixture separations, purification methods and characterization steps of organic compounds.

### Course Outcomes

After completion of this Course, the learner will be able to

1. apply theoretical concepts of coordination chemistry to synthesize inorganic complex compounds.
2. get knowledge of instrumental techniques, appropriate skillful handling of instruments, representation of data and interpretation of graphical results.
3. learn determination of chemical types of different organic binary mixture.
4. learn to separate solid organic binary mixtures on the basis of solubility.
5. learn to purify the separated organic compound by recrystallization technique.
6. learn characterization steps of organic compounds

<b>Course Code:</b> <b>CHEM 50811/</b> <b>CHEM 50812</b>	<b>Elective Practical: Chemistry Practicals</b> <b>Course Title: - Inorganic Chemistry and Organic Chemistry</b>	<b>Credits</b> <b>02</b>
	<b>Inorganic Chemistry</b>	<b>01</b>
	<b>Inorganic Preparations (Synthesis and Characterization)</b> 1) Bis-(tetramethylammonium) tetrachloro Cuprate (II) $(\text{Me}_4\text{N})_2[\text{CuCl}_4]$ 2) Bis-(tetramethylammonium) tetrachloro Nickelate (II) $(\text{Me}_4\text{N})_2[\text{NiCl}_4]$ 3) Bis (ethylenediammine) Copper (II) Sulphate $[\text{Cu}(\text{en})_2]\text{SO}_4$ 4) Hexaaamine Ni(II) Sulfate $[\text{Ni}(\text{NH}_3)_6]\text{SO}_4$ 5) Potassium trioxalato Chromate(III) $\text{K}_3[\text{Cr}(\text{C}_2\text{O}_4)_3]$ 6) Tetrammine monocarbanato Cobalt (III) Nitrate $[\text{Co}(\text{NH}_3)_4\text{CO}_3]\text{NO}_3$ <b>Instrumentation</b> 1) Determination of equilibrium constant by Slope intercept method for $\text{Fe}^{+3}/\text{SCN}^-$ system 2) Determination of Electrolytic nature of inorganic compounds by Conductance measurement.	
	<b>Physical Chemistry</b>	<b>01 Credit</b>
	<b>Non – Instrumental:</b> 1. Polar plots of atomic orbitals such as $1s$ , $2p_z$ and $3d_{z^2}$ orbitals by using angular part of hydrogen atom wave functions. 2. To study the influence of ionic strength on the base catalysed hydrolysis of ethyl acetate. 3. To study phase diagram of three component system water – chloroform /toluene - acetic acid. 4. To determine the rate constant of decomposition reaction of diacetone alcohol by dilatometric method.  <b>Instrumental:</b> 1. To determine the formula of silver ammonia complex by potentiometric method.  2. To determine CMC of sodium Lauryl Sulphate from measurement of conductivities at different concentrations. 3. To determine Hammett constant of <i>m</i> - and <i>p</i> - amino	

	benzoic acid/nitro benzoic acid by pH measurement. 4. To determine the Michaelis – Menten’s constant value (Km) of the enzyme Beta Amylase spectrophotometrically	
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**Reference:**

1. Advanced experiments in Inorganic Chemistry., G. N. Mukherjee., 1st 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: Dr Deepak

<b>PROGRAM(s): M.Sc-I</b>		<b>SEMESTER: II</b>			
<b>Course: Industrial Training/ Field Projects</b>		<b>Course Code: CHEM 512</b>			
<b>Teaching Scheme</b>					<b>Evaluation Scheme</b>
<b>Lectures (Hours per week)</b>	<b>Practical (Hours per week)</b>	<b>Tutorial (Hours per week)</b>	<b>Credit</b>	<b>Continuous Assessment (CA) (Marks-50)</b>	<b>Semester End Examination (Marks-50)</b>
NA	08	–	04	50	50
<p><b>Learning Objectives:</b>          To provide students the opportunity to test their interest in a particular career before permanent commitments are made.          To develop skills in the application of theory to practical work situations. To develop skills and techniques directly applicable to their careers.</p>					
<p><b>Course Outcomes:</b>  <b>At the end of the Course,</b>          Understand the Organizational Structure of a company.          Develop work habits and attitudes necessary for job success (technical competence, professional attitude, organization skills etc.)          Develop written communication and technical report writing skills.</p>					

**Proposed Structure of Assessment**  
**Theory Examination Pattern:**  
**A. Internal Assessment- 50%- 50 Marks per paper**

Sr.No.	Evaluation Type	Marks
1	Written Objective/Short Answer Examination	25
2	Assignment/ Case study/ field visit report/ presentation/ project	25
	Total	50

**External Examination- 50%-**

50 Marks per paper Semester End Theory Examination:  
Duration - These examinations shall be of two hours duration.

**Theory question paper pattern:**

There shall be 05 questions each of 10 marks on each unit.  
All questions shall be compulsory with internal choice within the questions.

**Paper Pattern:**

Question	Options	Marks	Questions Based on
Q.1	2 out of 4	10	Unit I
Q.2	2 out of 4	10	Unit II
Q.3	2 out of 4	10	Unit III
Q.4	2 out of 4	10	Unit IV
Q.5	5 out of 8	10	Units (I+II+III+IV)
	TOTAL	50	

**Semester End Practical Examination:**

Particulars	Continuous assessment (CA)	Semester end external examination
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<b>Laboratory work</b>	15	15
<b>Viva</b>	05	05
<b>Journal</b>	<b>05</b>	<b>05</b>
<b>Total</b>	<b>25</b>	<b>25</b>

### **PRACTICAL BOOK/JOURNAL**

The students are required to perform 75% of the Practical for the journal to be duly certified. The students are required to present a duly certified journal for appearing at the practical examination, failing which they will not be allowed to appear for the examination.