AC – ----------
ItemNo. ……..

University of Mumbai

M.Sc. Organic Chemistry Semester I & II CHOICE BASED (REVISED SYLLABUS) As Per NEP 2020 With Effect From The Academic Year 2023–2024

UNIVERSITY OF MUMBAI

Syllabus for Approval

Sr.No	Heading	Particulars
1	**Heading**	**Particulars**
2	Title of the Course	**M.Sc. Organic Chemistry**
3	Eligibility for Admission	B.Sc. Chemistry or equivalent qualification from other universities as may have been allowed by the relevant ordinances of this university
4	Passing Marks	40%
5	Ordinances / Regulations (if any)	
6	No. of Years / Semesters	Two
7	Level	PG
8	Pattern	Semester
9	Status	Revised

Date: Signature

Chairman
BoS in Chemistry

Dean,
Science and Technology

University of Mumbai

Credit Distribution Structure for Two Years

(M.Sc. in Organic Chemistry)

<table>
<tr><th rowspan="2">Year</th><th rowspan="2">Level</th><th rowspan="2">Sem</th><th colspan="2">Major</th><th rowspan="2">RM</th><th rowspan="2">OJT/ FP</th><th rowspan="2">RP</th><th rowspan="2">Cum. Cr.</th><th rowspan="2">Degree</th></tr>
<tr><th>Mandatory</th><th>Electives</th></tr>
<tr><td rowspan="7">1</td><td rowspan="7">6.0</td><td rowspan="5">Sem I</td><td>3×4+ 2=14</td><td>4</td><td>4</td><td rowspan="5">--</td><td rowspan="5">--</td><td rowspan="5">22</td><td rowspan="7">PG Diploma (after 3 Years Degree)</td></tr>
<tr><td>Inorganic Chemistry-I (CHEM 502)
Organic Chemistry-I (CHEM 503)
Analytical Chemistry-I (CHEM 505)
Chemistry Practical-I (Organic Chemistry and Analytical Chemistry) (PRCHEMOA 504)</td><td>Credits 4 (2+2)
Course 1 :
Physical Chemistry-I + Chemistry Practicals (Physical Chemistry and Inorganic Chemistry) (CHEM 50111)
(OR)
Credits 4 (2+2)
Course 2 :
Physical Chemistry-II + Chemistry Practicals (Physical Chemistry and Inorganic Chemistry) (CHEM 50112)</td><td>Research Methodology (CHEM 506)</td></tr>
<tr><td rowspan="5">Sem II</td><td>3*4+ 2=14</td><td>4</td><td rowspan="5">--</td><td rowspan="5">4 CHEM 512</td><td rowspan="5">--</td><td rowspan="5">22</td></tr>
<tr><td>Inorganic Chemistry-II (CHEM 508)
Organic Chemistry - II (CHEM 509)
Analytical Chemistry - II (CHEM 510)
Chemistry Practical-II (Organic Chemistry and Analytical Chemistry) (PRCHEMOA 511)</td><td>Credits 4 (2+2)
Course 1 :
Physical Chemistry-III + Chemistry Practicals (Physical Chemistry and Inorganic Chemistry) (CHEM 50711)
(OR)
Credits 4 (2+2)
Course 2 :
Physical Chemistry-IV + Chemistry Practicals (Physical Chemistry and Inorganic Chemistry) (CHEM 50712)</td><td>-----
PG Degree (after 3 Years Degree)</td></tr>
<tr><td colspan="2">Cum. Cr. For PG Diploma</td><td>28</td><td>8</td><td>4</td><td>4</td><td></td><td>44</td><td></td></tr>
<tr><td colspan="10">Exit Option: PG Diploma (44 credits) after Three Year UG Degree</td></tr>
</table>

M.Sc. Organic Chemistry

PROGRAM OUTLINE

YEAR		COURSE CODE	COURSE TITLE	CREDITS	Page Number
M.Sc. Sem-I	Mandatory Course-I	CHEM 502	Inorganic Chemistry-I	04	6
	Mandatory Course-II	CHEM 503	Organic Chemistry-I	04	11
	Mandatory Course-III	CHEM 505	Analytical Chemistry-I	04	15
	Mandatory Course Practical	PRCHEMOA 504	Chemistry Practical-I (Organic and Analytical Chemistry)	02	20
	Elective 1	CHEM 50111	Physical Chemistry-I and Chemistry Practical (Physical and Inorganic Chemistry)	04	22
	Elective 2	CHEM 50112	Physical Chemistry-II and Chemistry Practical (Physical and Inorganic Chemistry)	04	28
	RM	CHEM 506	Research Methodology	04	34
M.Sc. Sem-II	Mandatory Course-I	CHEM 508	Inorganic Chemistry-II	04	36
	Mandatory Course-II	CHEM 509	Organic Chemistry-II	04	40
	Mandatory Course-III	CHEM 510	Analytical Chemistry-II	04	44
	Mandatory Course Practical	PRCHEMOA 511	Chemistry Practical-II (Organic and Analytical Chemistry)	02	48
	Elective 1	CHEM 50711	Physical Chemistry-III and Chemistry Practical (Physical and Inorganic Chemistry)	04	50
	Elective 2	CHEM 50712	Physical Chemistry-IV and Chemistry Practical (Physical and Inorganic Chemistry)	04	56
	OJT/FP	CHEM 512	Industrial Training/Field Project	04	62
			Proposed Examination Pattern		63

PROGRAMME SPECIFIC OUTCOME (PSOs)

1. Gain knowledge of the advanced concepts in the branch of chemistry, scrutinize and accomplish a solution to problems encountered in the field of research and analysis.

2. Apply the basic knowledge of chemistry to perform various tasks assigned to them at the workplace in industry and academia to meet the global standards.

3. Deduce qualitative and quantitative information of chemical compounds using advanced spectroscopic methods which can further be analysed using practical skills inculcated in them during the course.

4. Imbibe the attitude as well as aptitude of a scientific approach along with analytical reasoning with respect to the novel techniques actually implemented in the Industry.

5. Use the subject knowledge, communication and ICT skills to become an effective team leader/team member in the interdisciplinary fields.

6. Understand, Manage and contribute to solve basic societal issues and environmental concerns ethically based on principles of scientific knowledge gained.

7. Exhibit professional work ethics and norms of scientific development.

PROGRAM(s): M.Sc.-I		SEMESTER: I			
Course:Paper-I		Course Code: (CHEM502) Course Title:- Inorganic Chemistry-I			
Teaching Scheme					Evaluation Scheme
Lectures (Hours per week)	Practical (Hours per week)	Tutorial (Hours per week)	Credit	Continuous Assessment (CA) (Marks- 50)	Semester End Examination (Marks- 50)
04	NA	–	04	50	50

Learning Objectives:

Inorganic Chemistry

1. To develop the ability to correlate fundamental theories of spatial orientations of molecules based on wave mechanics with advancedconceptsin chemical bonding ,symmetry of molecular systems and Structural aspects of inorganic solids.
2. To gain theoretical knowledge of cutting edge topics such as solid state lasers and contemporary Methods of preparation of nanomaterial's .
3. To learn about diverse tools available for characterization of coordination compounds in order to enhance competency while applying for practical purpose

Course Outcomes:

1. The learner will know the important fundamental concept of Group Theory, which helps them in understanding the properties and bonding in polyatomic molecules.
2. The learner get the knowledge about the various techniques used for Characterization coordination compounds.
3. The learners develops the skill in interpretation of the spectra.
4. Thelearnerswill get comprehensive idea about established instrumental techniques and Significant characterization tools available to study inorganic complexes having wide applications in industries.

Course Code : (CHEM 502)

Course Title:-Inorganic Chemistry-I

Unit – I

Unit I Chemical Bonding: [15 L]

1.1 Recapitulation of hybridization Derivation of wave functions for sp, sp2, sp3 orbital hybridization types considering only sigma bonding.

1.2 Discussion of involvement of d orbitals in various types of hybridizations. Concept of resonance, resonance energy derivation expected. Formal charge with examples.

1.3 Molecular Orbital Theory for diatomic species of First transition Series.

1.4 Molecular Orbital Theory for Polyatomic species considering σ bonding for SF6, CO2, B2H6, I3 - molecular species.

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.

Unit II

Molecular Symmetry and Group Theory: [15L]

2.1. Symmetry criterion of optical activity, symmetry restrictions on dipole moment. A systematic procedure for symmetry classification of molecules.

2.2. Concepts of Groups, Sub-groups, Classes of Symmetry operations, Group Multiplication Tables. Abelian and non-Abelian point groups.

2.3.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 C2v, C3v and C2h, structure of character tables.

b) Determination of symmetry species for translations and rotations.

c) Mulliken‟s notations for irreducible representations.

d) Reduction of reducible representations using reduction formula.

2.4. Applications of Group Theory Symmetry adapted linear combinations (SALC), symmetry aspects of MO theory, sigma bonding in ABn (NH3, CH4) molecule.

Unit III

Materials Chemistry and Nanomaterials: [15 L]

3.1 Solid State Chemistry -

3.1.1. Electronic structure of solids and band theory, Fermi level, K Space and Brillouin Zones.

3.1.2. Structures of Compounds of the type: AB [nickel arsenide (NiAs)], AB2 [fluorite (CaF2) and anti-fluorite structures, rutile (TiO2)

3.1.3. Solid state lasers: Introduction, Types, Working & Applications

3.2 Nanomaterials-

3.2.1 Preparative methods, Chemical methods, solvothermal, combustion synthesis, microwave, coprecipitation, Langmuir-Blodgett(LB) method, biological methods, synthesis using microorganism.

3.2.2 Applications in the field of semiconductors, solar cells.

Unit IV

Characterization of Coordination compounds [15L]

4.1. Methods of Characterization: thermal studies, Conductivity measurements, electronic spectral and magnetic measurements, IR, NMR and ESR spectroscopic methods.

4.2. Introduction to Orgel& Tanabe Sugano Diagram, Terms, Splitting of terms in Octahedral weak field, Calculation of electron parameters Δ, β, C and Nephlauxetic ratio with suitable examples.

4.3. Determination of formation constants of metal complexes (Overall and Stepwise): Comparative studies of Potentiometric and spectrophotometric methods.

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. SalahuddinKunju 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*, 7th Edn., Oxford University Press, 2002.
8.An introduction to Lasers Theory and Applications by M.N. Avadhanulu,P.S.Hemne, S.Chand publication.
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 & 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
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).

PROGRAM(s): M.Sc.-I	SEMESTER: I				
Course: Paper-II	Course Code: (CHEM 503) Course Title:- Organic Chemistry-I				
Teaching Scheme					Evaluation Scheme
Lectures (Hours per week)	Practical (Hours per week)	Tutorial (Hours per week)	Credit	Continuous Assessment (CA) (Marks- 50)	Semester End Examination (Marks- 50)
04	NA	–	04	50	50

Learning Objectives:

1.To enable learners to have comprehensive knowledge and understanding of the advanced concepts in reaction Mechanism, stereochemistry, different reactions and reagents.

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.

3. Accomplish a solution to problems encountered in the field of research.

Course Outcomes:

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)

Course Title:-Organic Chemistry-I

Unit I

Physical Organic Chemistry: (15L)

1.1. Thermodynamic and kinetic requirements of a reaction: rate and equilibrium constants, reaction coordinate diagram, transition state (activated complex), nature of activated complex, Hammond postulate, Reactivity *vs* selectivity, Curtin-Hammett Principle, Microscopic reversibility, Kinetic *vs* thermodynamic control of organic reactions.

1.2. Determining mechanism of a reaction: Product analysis, kinetic studies, use of isotopes (Kinetic isotope effect – primary and secondary kinetic isotope effect). Detection and trapping of intermediates, crossover experiments and stereochemical evidence.

1.3. Acids and Bases: Factors affecting acidity and basicity: Electronegativity and inductive effect, resonance, bond strength, electrostatic effects, hybridization, aromaticity and solvation. Comparative study of acidity and basicity of organic compounds on the basis of pKa values, Leveling effect and non-aqueous solvents. Acid and base catalysis – general and specific catalysis with examples.

Unit-II

Stereochemistry: (15 L)

2.1. Concept of Chirality: Recognition of symmetry elements.

2.2. Molecules with tri- and tetra-coordinate centers: Compounds with carbon, silicon, nitrogen, phosphorous and sulphur chiral centers, relative configurational stabilities.

2.3. Molecules with two or more chiral centers: Constitutionally unsymmetrical molecules: erythro-threo and syn-anti systems of nomenclature. Interconversion of Fischer, Sawhorse, Newman and Flying wedge projections. Constitutionally symmetrical molecules with odd and even number of chiral centers: enantiomeric and meso forms, concept of stereogenic, chirotopic, and pseudoasymmetriccentres. R-S nomenclature for chiral centres in acyclic and cyclic compounds.

2.4. Axial and planar chirality: Principles of axial and planar chirality. Stereochemical features and configurational descriptors (R,S) for the following classes of compounds: allenes, alkylidene cycloalkanes, spirans, biaryls (buttressing effect) (including BINOLs and BINAPs), ansa compounds, cyclophanes, trans-cyclooctenes.

2.5. Prochirality: Chiral and prochiralcentres; prochiral axis and prochiral plane. Homotopic, heterotopic (enantiotopic and diastereotopic) ligands and faces.Identification using substitution and symmetry criteria.Nomenclature of stereoheterotopic ligands and faces. Symbols for stereoheterotopic ligands in molecules with i) one or more prochiralcentres ii) a chiral as well as a prochiralcentre, iii) a prochiral axis iv) a prochiral plane v) pro-pseudoasymmetriccentre. Symbols for enantiotopic and diastereotopic face.

Unit III

Nucleophilic substitution reactions and Aromaticity (15L)

3.1. Nucleophilic substitution reactions: (9 L)

3.1.1 Aliphatic nucleophilic substitution: S_N1, S_N2, S_N^i reactions, mixed S_N1 and S_N2 and SET mechanisms. S_N reactions involving NGP - participation by aryl rings, σ and pi-bonds. Factors affecting these reactions: substrate, nucleophilicity, solvent, steric effect, hard-soft interaction, leaving group. Ambident nucleophiles. $S_{NC}A$, S_N1‟ and S_N2‟ reactions. S_N at sp^2 (vinylic) carbon.

3.1.2 Aromatic nucleophilic substitution: S_NAr, S_N1, benzyne mechanisms. Ipso, cine, tele and vicarious substitution.

3.1.3 Ester hydrolysis: Classification, nomenclature and study of all eight mechanisms of acid and base catalyzed hydrolysis with suitable examples.

3.2. Aromaticity: (6 L)

3.2.1. Huckel's (4n+2) and 4n rules, structural, thermochemical, and magnetic criteria for aromaticity, including NMR characteristics of aromatic systems. Delocalization and aromaticity.

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 (C_{60}).

Unit-IV

Oxidation and Reduction: (15L)

4.1. Oxidation: General mechanism, selectivity, and important applications of the following:

4.1.1. Dehydrogenation: Dehydrogenation of C-C bonds including aromatization of six membered rings using metal (Pt, Pd, Ni) and organic reagents (chloranil, DDQ).

4.1.2. Oxidation of alcohols to aldehydes and ketones: Chromium reagents such as $K_2Cr_2O_7/H_2SO_4$ (Jones reagent), CrO_3-pyridine (Collin's reagent), PCC (Corey's reagent) and PDC (Cornforth reagent), hypervalent iodine reagents (IBX, Dess-Martin periodinane). DMSO based reagents (Swern oxidation), Corey-Kim oxidation - advantages over Swern and limitations; and Pfitzner-Moffatt oxidation-DCC and DMSO and Oppenauer oxidation.

4.1.3. Oxidation involving C-C bonds cleavage: Glycols using HIO_4; cycloalkanones using CrO_3; carbon-carbon double bond using ozone, $KMnO_4$, CrO_3, $NaIO_4$ and OsO_4; aromatic rings using RuO_4 and $NaIO_4$.

4.1.4. Oxidation involving replacement of hydrogen by oxygen: oxidation of CH_2 to CO by SeO_2, oxidation of arylmethanes by CrO_2Cl_2 (Etard oxidation).

4.1.5. Oxidation of aldehydes and ketones: with H_2O_2 (Dakin reaction), with peroxy acid (Baeyer-Villiger oxidation)

4.2. Reduction: General mechanism, selectivity, and important applications of the following reducing reagents:

4.2.1. Reduction of CO to CH_2 in aldehydes and ketones-Clemmensen reduction, Wolff-Kishner reduction and Huang-Minlon modification.

4.2.2. Metal hydride reduction: Boron reagents ($NaBH_4$, $NaCNBH_3$, diborane, 9-BBN, $Na(OAc)_3BH$, aluminium reagents ($LiAlH_4$, DIBAL-H, Red Al, L and K- selectrides).

4.2.3. N_2H_2 (diimide reduction) and other non-metal based agents including organic reducing agents (Hantzschdihydropyridine).

4.2.4. Dissolving metal reductions: using Zn, Li, Na, and Mg under neutral and acidic conditions, Li/Na-liquid NH_3 mediated reduction of aromatic compounds (Birch reduction) and Alkynes.

Reference Books.

1. Physical Organic Chemistry, NeilIsaacs
2. Modern Physical Organic Chemistry, Eric V. Anslynand Dennis A.Dougherty
3. Comprehensive Organic chemistry, Barton and Ollis,Vol1
4. Organic Chemistry, J. Claydens, N. Greeves, S.Warren and P. Wothers, Oxford University Press.
5. Advanced Organic Chemistry, F.A. Careyand R.J. Sundberg, Part A and B, Plenum Press.
6. Stereochemistry: Conformation and mechamism, 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. Millerand R.Prasad, Pearson Education.
11. Advanced Organic Chemistry: Reaction mechanisms, R. Bruckner,AcademicPress.
12. Understanding Organic Reaction Mechanisms, Adams Jacobs, Cambridge University Press.
13. Writing Reaction Mechanism inorganic 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, 6^{th} 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. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Nelson Thornes

PROGRAM(s): M.Sc.-I	SEMESTER: I				
Course: Paper-III	Course Code: (CHEM 505) Course Title:- Analytical Chemistry-I				
Teaching Scheme					Evaluation Scheme
Lectures (Hours per week)	Practical (Hours per week)	Tutorial (Hours per week)	Credit	Continuous Assessment (CA) (Marks- 50)	Semester End Examination (Marks- 50)
04	NA	–	04	50	50

Learning Objectives:

1. To enable learners to have comprehensive knowledge, understanding of the types of instruments with operations and automated methods of analysis.
2. To apply the basic knowledge of quality systems, quality audit and quality managements,.
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.
4. To provide solutions to problems encountered in the field of analysis and research.

Course Outcomes:

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

1. Understand various terms used in analytical chemistry.
2. Identify the different types of errors in analysis.
3. Sketch out the role and importance of total quality management, safety, accreditations 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. transformation reaction.

Course Code : (CHEM 505)

Course Title:- Analytical Chemistry-I

Unit - I

1.1 Language of Analytical Chemistry [8 L]

1.1.1 Analytical perspective [3 L]

Analytical approach.common analytical problems. Terms involved in analytical chemistry - Analysis, Analyte, Matrix, Determination, Measurement, Techniques, Methods, Procedures and protocol.

1.1.2 An overview of analytical methods [3 L]

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.

1.1.3 Errors [2 L]

Types of errors.Absolute error, Relative error, Constant error and Proportionate errors.Minimization of errors.

1.2 Quality in Analytical Chemistry [7L]

1.2.1 Total Quality Management- TQM [3L]

Definition, Principles, Importance and benefits. Philosophy of implementation of TQM - Process steps, Advantages and Limitations **i)** Kaizen -Six steps **ii)** Six Sigma approach **iii)** 5S and 5S audit check for laboratories.

1.2.2 Safety in laboratories [2L]

Basic concept of safety in laboratory- The Industrial Hygiene Principles.Personal protection equipment (PPE).Occupational Safety and Health Administration (OSHA).

1.2.3 Accreditations [2L]

Accreditation of laboratories, NABL**,** Indian Government standards (ISI, HALLMARK, AGMARK).- Meaning and significance.

Unit- II

2.1 Calculations based on Chemical Principles [15 L]

(The following topics are to be covered in the form of numerical problems only)

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

Unit III -Optical Methods [15 L]

3.1 Infrared Absorption Spectroscopy [6 L]

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.

3.2 FT Technique [3 L]

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.

3.3 Molecular Ultraviolet and Visible Spectroscopy [6 L]

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:

i) On charge transfer absorption
ii) Simultaneous spectroscopy
iii) Derivative Spectroscopy

3.3.3 Dual spectrometry – Introduction, Principle, Instrumentation and Applications**.**

Unit - IV Instrumental methods-I [15L]

4.1 Thermal Methods: [9 L]

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.

4.2 Automation in chemical analysis: [6 L]

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 systems, 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, 5th Edition, Ch: 1
3. Fundamentals of Analytical Chemistry, Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, 9th Edition, 2004, Ch: 5.
4. Undergraduate Instrumental Analysis ; J W Robinson, Marcel Dekker, 6th edition Ch:1.
5. ISO 9000 Quality Systems Handbook; David Hoyle. 4th 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; Andreae, 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, 5th 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 th 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. TheophanidesTheophile (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

PROGRAM(s): M.Sc.-I		SEMESTER: I			
Course: Practical		Course Code: PRCHEMOA504 Course Title:- Chemistry Practical-I (Organic Chemistry and Analytical Chemistry)			
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)
NA	04	NA	02	50	50

Learning points:

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

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

1. Carry out one step preparation in laboratory with basic understanding of stoichiometry
2. Evaluate the process and outcomes of an experiment quantitatively and qualitatively
3. Check purity of product using thin layer chromatography
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

Course Code: PRCHEMOA 504

Organic Chemistry Practicals

One step preparations (1.0 g scale)

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

(Minimum 08 experiments are expected)

Analytical Chemistry Practicals

Instrumental Experiments

1. To determine percentage purity of sodium carbonate in washing soda pH metrically.
2. To determine amount of Ti(III) and Fe(II) in a mixture by titration with Ce(IV)potentiometrically.
3. To determine the percentage purity of a sample (glycine/sodium benzoate/primary amine) by titration with perchloric acid in a non-aqueous medium using glass calomel system potentiometrically.
4. To determine the amount of nitrite present in the given water sample colorimetrically.

Non-Instrumental Experiments

1.To carry out assay of the sodium chloride injection by Volhard's method.

2.To determine (a) the ion exchange capacity (b) exchange efficiency of the given cation exchange resin.

3.To determine amount of Cr(III) and Fe(II) individually in a mixture of the two by titration with EDTA.

4.To determine number of nitro groups in the given compound using$TiCl_3$.

References:

1. Quantitative Inorganic Analysis including Elementary Instrumental Analysis by ; A. I. Vogels, 3rd Ed. ELBS (1964)
2. Vogel's textbook of quantitative chemical analysis, Mendham, Denny, Barnes, Thomas, Pearson education, Sixth Ed.
3. Standard methods of chemical analysis ; F. J. Welcher, 1975
4. Standard methods of chemical analysis :Instrumental methods of Analysis ; F. J. Welcher , vol. 3, 1966
5. "Standard methods of Chemical Analysis"; W. W. Scott, Vol. I, Van Nostrand Company, Inc.,1939.
6."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 50111)
Course Title:- Physical Chemistry Elective- I

PROGRAM(s): M.Sc.-I		**SEMESTER: I**			
Course: Elective:I		**Course Code: (CHEM50111)** **Course Title:- Physical Chemistry-I**			
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**	**50**	**50**

Learning Objectives:

Physical Chemistry

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.

Course Outcomes:

1. The learners will apply the advanced thermodynamics, Maxwell equation and its applications to ideal gasses.
2. The learners will implement the applications of chemical thermodynamics to real gases, solutions, surfaces and their energetics.
3. The learners will understand the applications of operators and Schrodinger equation in the field of quantum Chemistry.
4. The learners will try to accomplish a solution to problems encountered in the field of research.

Elective: I Physical Chemistry-I

Unit - I

Thermodynamics-I [15]

1.1.State function and exact differentials. Maxwell equations, Maxwell thermodynamic Relations; it‟s significance and applications to ideal gases, Joule Thomson experiment, Joule Thomson coefficient, inversion temperature, Joule Thomson coefficient in terms of van der Waals constants. **[8L]**

1.2.Third law of Thermodynamics, Entropy change for a phase transition, absolute entropies, determination of absolute entropies in terms of heat capacity, standard molar entropies and their dependence on molecular mass and molecular structure, residual entropy. **[7L]** [Ref 2 and 1,10,11,12 17]

Unit II

Quantum Chemistry: [15L]

2.1.Classical Mechanics, failure of classical mechanics: Need for Quantum Mechanics.

2.2.Particle waves and Schrödinger wave equation, wave functions, properties of wave functions, Normalization of wave functions, orthogonality of wave functions.

2.3.Operators and their algebra, linear and Hermitian operators, operators for the dynamic variables of a system such as, position, linear momentum, angular momentum, total energy, eigen functions, eigen values and eigen value equation, Schrödinger wave equation as the eigen value equation of the Hamiltonian operator, average value and the expectation value of a dynamic variable of the system, Postulates of Quantum Mechanics, Schrodinger‟s Time independent wave equation from Schrodinger‟s time dependent wave equation.

2.4.Application of quantum mechanics to the following systems:

a) Free particle, wave function and energy of a free particle.
b) Particle in a one, two and three dimensional box, separation of variables, Expression for the wave function of the system, expression for the energy of the system, concept of quantization, introduction of quantum number, degeneracy of the energy levels.
c) Harmonic oscillator, approximate solution of the equation, Hermite polynomials, expression for wave function, expression for energy, use of the recursion formula.

[Ref 7, 8 and 9]

References: (Elective:I and II)

1. Peter Atkins and Julio de Paula, Atkin‟s*Physical Chemistry*, 7thEdn., Oxford University Press, 2002.
2. K.J. Laidler and J.H. Meiser, *Physical Chemistry*, 2nd Ed., CBS Publishers and Distributors, New Delhi, 1999.
3. Robert J. Silby and Robert A. Alberty, *Physical Chemistry*, 3rdEdn., John Wiley and Sons (Asia) Pte. Ltd., 2002.
4. Ira R. Levine, *Physical Chemistry*, 5thEdn., Tata McGraw-Hill New Delhi, 2002.
5. G.W. Castellan, *Physical Chemistry*, 3rdEdn.,Narosa Publishing House, New Delhi, 1983.
6. S. Glasstone, *Text Book of Physical Chemistry*, 2ndEdn., McMillan and Co. Ltd., London, 1962
7. B.K. Sen, *Quantum Chemistry including Spectroscopy*, Kalyani Publishers, 2003.
8. A.K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw – Hill, 1994.
9. R.K. Prasad, *QuantumChemistry*, 2ndEdn., New Age International Publishers, 2000.
10. S. Glasstone, *Thermodynamics for Chemists*, Affiliated East-West Press, New Delhi, 1964.
11. W.G. Davis, *Introduction to Chemical Thermodynamics – A Non – Calculus Approach*, Saunders, Philadelphia, 19772.
12. Peter A. Rock, *Chemical Thermodynamics*, University Science Books, Oxford University Press, 1983.
13. Ira N. Levine, *Quantum Chemistry*, 5thEdn., Pearson Education (Singapore) Pte. Ltd., Indian Branch, New Delhi, 2000.
14. Thomas Engel and Philip Reid, Physical Chemistry, 3rdEdn., Pearson Education Limited 2013.
15. D.N. Bajpai, Advanced Physical Chemistry, S. Chand 1stEdn., 1992.
16. ***Bockris***, John O'M., ***Reddy***, Amulya K.N., Gamboa-Aldeco, Maria E., Modern Electrochemistry, 2A, Plenum Publishers, 1998.
17. Physical Chemistry by Gurtu and Gurtu.
18. Dr. Harichandra A Parbat and Dr. Damodar V Prabhu, Essence of Chemical Kinetics, Sara Publication, First Edition, Sept. 2022.
19. A Text book of Physical Chemistry by K L kapoor Vol 5 , 2ndEdn

Elective Practical I

PROGRAM(s): M.Sc.-I		SEMESTER: I			
Course: Practical		Course Code: CHEM50111 Course Title:- Physical and Inorganic Chemistry Practical-I			
Teaching Scheme					Evaluation Scheme
Lectures (Hours per week)	Practical (Hours per week)	Tutorial(Hours perweek)	Credit	Continuous Assessment (CA)	Semester End Examination
02	NA	–	02	25	25

Learning Objectives:

Physical Chemistry

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 usage of subject fundamentals-principles with practical knowledge to design experiments, analyze and interpret data so as to reach to proper conclusions.

5.Learner will train the handling of equipments like potentiometer, conductivity meter, colorimeter and spectrophotometer.

6. Learner will develop scientific temper and research based skills accomplish to encountered in the field of research.

Inorganic Chemistry

1. To apply basic concepts of separation and estimation of metals ions from constituent ores/alloys effectively using chemical analysis
2. To gain knowledge of employing instrumental techniques for quantitative analysis.
3. The learner can able to analyze structure, reactivity and reaction mechanisms of coordination compounds.
4. It explains various methods, concepts, highlights on effect of environment on human beings.
5. Will able to understand Commercial applications of novel materials in synthesis of compounds.

Chemistry Practical-I

Course Code: CHEM 50111

Non – Instrumental:

1.To determine the heat of solution (ΔH) of a sparingly soluble acid (benzoic/salicylic acid) from solubility measurement at three different temperature.
2.To study the variation of calcium sulphate with ionic strength and hence determine the thermodynamic solubility product of $CaSO_4$ at room temperature.
3.To investigate the reaction between acetone and iodine.
4.Graph Plotting of mathematical functions –linear, exponential and trigonometry and identify whether functions are acceptable or non-acceptable?

Instrumental:

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.

References:

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

Inorganic Chemistry Practical
Course Code: CHEM 50111

Ores and Alloys

1) Analysis of Devarda‟s alloy
2) Analysis of Cu – Ni alloy
3) Analysis of Limestone.
4) Analysis of Tin Solder alloy

Instrumentation

1) Estimation of Fe (III)solution using Ce (IV) ions Potentiometrically
2) Estimation of Copper using Iodometric method Potentiometrically
3) Estimation of Na_2CO_3 in washing soda by pH metry
4) Estimation of Cl- ion in NaCl/KCl by Conductometry.

Reference:

1. Advanced experiments in Inorganic Chemistry., G. N. Mukherjee., 1st Edn., 2010., U.N.Dhuri& 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

Elective: II Physical Chemistry-II

PROGRAM(s): M.Sc.-I	SEMESTER: I
Course: Elective-II	Course Code: (CHEM50112) 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	50	50

Learning Objectives:

Physical Chemistry

1. 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.

Course Outcomes :

1. The learners evaluate the different theories of chemical kinetics and effect of temperature on reaction rates.
2. The learners will understand the applications of chain reactions in the field of Polymer Chemistry.
3. The learners will evaluate the resting membrane potential by using the concept of bio electrochemistry.
4. The learners will try to accomplish a solution to problems encountered in the field of research.

Course Code: (CHEM 50112)
Elective : II Physical Chemistry-II

Unit I

Chemical Kinetics and Molecular Dynamics-I [15L]

1.1.Composite Reactions:

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.

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.

1.3.Reaction in Gas Phase

Unimolecular Reactions: Lindeman-Hinshelwood theory, Rice-Ramsperger-Kasssel (RRK) theory, Rice-Ramsperger-Kassel Marcus (RRKM) theory.

[Ref. 2 and 15, 17, 18]

Unit II

Electrochemistry [15L]

Recapitulation – basics of electrochemistry.

2.1. Debye-Hückel theory of activity coefficient, Debye-Hückel limiting law and its extension to higher concentration (derivations are expected).

2.2. Electrolytic conductance and ionic interaction, relaxation effect,.Debye-Hückel-Onsager equation (derivation expected). Validity of this equation for aqueous and non- aqueous solution, deviations from Onsager equation, Debye - Falkenhagen effect (dispersion of conductance at high frequencies), Wien effect.

2.3. Batteries: Alkaline fuel cells, Phosphoric acid fuel cells, High temperature fuel cells [Solid –Oxide Fuel Cells (SOFC) and Molten Carbonate Fuel Cells]

2.4. Bio-electrochemistry: Introduction, cells and membranes, membrane potentials, theory of membrane potentials, interfacial electron transfer in biological systems, adsorption of proteins onto metals from solution, electron transfer from modified metals to dissolved protein in solution, enzymes as electrodes, electrochemical enzyme-catalysed oxidation of styrene. Goldmann equation. (derivations are expected)

[Ref: 14 and 16, 17, 18]

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

References: (Elective:I and II)

1. Peter Atkins and Julio de Paula, Atkin"s*Physical Chemistry*, 7thEdn., Oxford University Press, 2002.
2. K.J. Laidler and J.H. Meiser, *Physical Chemistry*, 2nd Ed., CBS Publishers and Distributors, New Delhi, 1999.
3. Robert J. Silby and Robert A. Alberty, *Physical Chemistry*, 3rdEdn., John Wiley and Sons (Asia) Pte. Ltd., 2002.
4. Ira R. Levine, *Physical Chemistry*, 5thEdn., Tata McGraw-Hill New Delhi, 2002.
5. G.W. Castellan, *Physical Chemistry*, 3rdEdn.,Narosa Publishing House, New Delhi, 1983.
6. S. Glasstone, *Text Book of Physical Chemistry*, 2ndEdn., McMillan and Co. Ltd., London, 1962
7. B.K. Sen, *Quantum Chemistry including Spectroscopy*, Kalyani Publishers, 2003.
8. A.K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw – Hill, 1994.
9. R.K. Prasad, *QuantumChemistry*, 2ndEdn., New Age International Publishers, 2000.
10. S. Glasstone, *Thermodynamics for Chemists*, Affiliated East-West Press, New Delhi, 1964.
11. W.G. Davis, *Introduction to Chemical Thermodynamics – A Non – Calculus Approach*, Saunders, Philadelphia, 19772.
12. Peter A. Rock, *Chemical Thermodynamics*, University Science Books, Oxford University Press, 1983.
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14. Thomas Engel and Philip Reid, Physical Chemistry, 3rdEdn., Pearson Education Limited 2013.
15. D.N. Bajpai, Advanced Physical Chemistry, S. Chand 1stEdn., 1992.
16. ***Bockris***, John O'M., ***Reddy***, Amulya K.N., Gamboa-Aldeco, Maria E., Modern Electrochemistry, 2A, Plenum Publishers, 1998.
17. Physical Chemistry by Gurtu and Gurtu.
18. Dr. Harichandra A Parbat and Dr. Damodar V Prabhu, Essence of Chemical Kinetics, Sara Publication, First Edition, Sept. 2022.
19. A Text book of Physical Chemistry by K L kapoor Vol 5 , 2ndEdn

Elective Practical II

PROGRAM(s): M.Sc.-I		SEMESTER: I			
Course: Practical		Course Code: CHEM50112 Course Title:- Physical and Inorganic Chemistry Practical-I			
Teaching Scheme					Evaluation Scheme
Lectures (Hours per week)	Practical (Hours per week)	Tutorial (Hours per week)	Credit	Continuous Assessment (CA)	Semester End Examination
02	NA	–	02	25	25

Learning Objectives:

Physical Chemistry

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

Inorganic Chemistry

1. To apply basic concepts of separation and estimation of metals ions from constituent ores/alloys effectively using chemical analysis
2. To gain knowledge of employing instrumental techniques for quantitative analysis.
3. The learner can able to analyze structure, reactivity and reaction mechanisms of coordination compounds.
4. It explains various methods, concepts, highlights on effect of environment on human beings.
5. Will able to understand Commercial applications of novel materials in synthesis of compounds.

Elective Practical-II

Course Code: CHEM 50112

Physical Chemistry

Non – Instrumental:

1.To determine the heat of solution (ΔH) of a sparingly soluble acid (benzoic/salicylic acid) from solubility measurement at three different temperature.
2.To study the variation of calcium sulphate with ionic strength and hence determine the thermodynamic solubility product of $CaSO_4$ at room temperature.
3.To investigate the reaction between acetone and iodine.
4.Graph Plotting of mathematical functions –linear, exponential and trigonometry and identify whether functions are acceptable or non-acceptable?

Instrumental:

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.

References:

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

Elective Practical II
Course Code: CHEM 50112
Inorganic Chemistry

Ores and Alloys

1) Analysis of Devarda‟s alloy
2) Analysis of Cu – Ni alloy
3) Analysis of Limestone.
4) Analysis of Tin Solder alloy

Instrumentation

5) Estimation of Fe (III)solution using Ce (IV) ions Potentiometrically
6) Estimation of Copper using Iodometric method Potentiometrically
7) Estimation of Na_2CO_3 in washing soda by pH metry
8) Estimation of Cl- ion in NaCl/KCl by Conductometry.

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

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

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.

Research Methodology

Unit I Literature Survey

1.1 Print:

Primary, Secondary and Tertiary sources. Journals: Journal abbreviations, abstracts, current titles, 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.

1.2 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.

1.3 Information Technology and Library Resources:

The Internet and World wide web, Internet resources for Chemistry, finding and citing published information.

Unit II DATA ANALYSIS

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.

Unit III METHODS OF SCIENTIFIC RESEARCH AND WRITING SCIENTIFIC PAPERS

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.

Unit IV CHEMICAL SAFETY & ETHICAL HANDLING OF CHEMICALS

Safe working procedure and protective environment, 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.

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

PROGRAM(s): M.Sc.-I		SEMESTER: II			
Course:Paper-I		Course Code: (CHEM508) Course Title:- Inorganic Chemistry-II			
Teaching Scheme					Evaluation Scheme
Lectures (Hours per week)	Practical (Hours per week)	Tutorial (Hours per week)	Credit	Continuous Assessment (CA) (Marks- 50)	Semester End Examination (Marks- 50)
04	NA	–	04	50	50

Learning Objectives:

1. The course aims at the detailed mechanistic study of various inorganic complexes.
2. The course aims at the detailed interception of bonding concepts in organometallic and bioinorganic chemistry.
3. The course also aims at a detailed understanding of bio inorganic chemistry of metals.
4. The course also aims to study the preparation of different inorganic complexes.

Course Outcomes: The learners will be able to study rates of reactions and the factors affecting them and understand the different techniques used to study the rate of the reaction.

1. The learners will be able to learn ligand substitution reactions of Octahedral and Square planar complexes, Trans effect and factors affecting these substitution reactions.

2. The learners will be able to understand the 18 e^- and 16 e^- electron square planar complexes by studying different examples. They will also learn the preparation and properties of a few selected compounds including sandwich compounds of Fe, Cr

3. The learners will understand the structure and bonding of a few inorganic compounds like Ziese's salt, ferrocene and bis(arene)chromium(0)

4. The learners will understand the occurrence and effect of toxic metals like Pb, As, Cu, Cd, and Hg on the environment, the different diseases caused by poisoning of metals and the impact these metals have on the living organism.

5. The learners will be familiar with the role of Inorganic chemistry in Biological systems, understand the structure of various biological oxygen carriers and molecules involved in electron storage and transport.

Course Code: (CHEM 508)

Course Title:-Inorganic Chemistry-II

Unit I

Inorganic Reaction Mechanism: [15 L]

1.1 Rate of reactions, factors affecting the rate of reactions, techniques for determination of rate of reaction (Direct chemical analysis, spectrophotometric method, electrochemical and flow methods).

1.2 Ligand substitution reactions of:

a) Octahedral complexes without breaking of metal-ligand bond (Use of isotopic

labelling method)

b) Square planar complexes, trans-effect, its theories and applications. Mechanism

and factors affecting these substitution reactions.

1.3 Redox reactions: inner and outer sphere mechanisms, complimentary and non-complimentary reactions.

1.4 Isomerization and racemization reactions

Unit II

Organometallic Chemistry of Transition metals: [15 L]

2.1. Eighteen electron rule & electron counting with examples, sixteen electron Square Planar complexes.

2.2. Preparation and properties of the following compounds

(a) Alkyl and aryl derivatives of Pd and Pt complexes

(b) Carbenes and carbynes of Cr, Mo and W

(c) Alkene derivatives of Pd and Pt

(d) Alkyne derivatives of Pd and Pt

(e) Allyl derivatives of nickel

(f) Sandwich compounds of Fe, Cr and Half Sandwich compounds of Cr, Mo.

2.3 Structure and bonding on the basis of VBT and MOT in the following organometallic compounds:

Zeise‟s salt, bis(triphenylphosphine)diphenylacetylene platinum (0) $[Pt(PPh_3)_2(HC{\equiv}CPh)_2]$, diallylnickel(diallylnickel(II), ferrocene and bis(arene)chromium(0), tricarbonyl (η^2-butadiene) iron(0).

Unit III

Environmental Chemistry: [15 L]

3.1. Conception of Heavy Metals: Critical discussion on heavy metals

3.2. Toxicity of metallic species: a) Mercury, lead, cadmium, arsenic, copper and chromium, with respect to their sources, distribution, speciation, biochemical effects and toxicology, control and treatment.

b) Itai-itai disease for Cadmium toxicity,

c) Arsenic Poisoning in the Indo-Bangladesh region.

3.3. Interaction of radiation in context with the environment: Sources and biological implication of radioactive materials. Effect of low-level radiation on cells- Its applications in diagnosis and treatment, Effect of radiation on cell proliferation and cancer.

Unit IV

Bioinorganic Chemistry: [15 L]

4.1. Biological oxygen carriers; hemoglobin, hemerythrene and hemocyanine- structure of metal active center and differences in mechanism of oxygen binding, Differences between hemoglobin and myoglobin: Cooperativity of oxygen binding in hemoglobin and Hill equation, pH dependence of oxygen affinity in hemoglobin and myoglobin and its implications.

4.2. Activation of oxygen in biological system with examples of mono-oxygenases

4.3. Copper containing enzymes- superoxide dismutase,

4.4. Nitrogen fixation-nitrogenase, hydrogenases

4.5. Metal ion transport and storage: Ionophores, transferrin, ferritin and metallothionins

4.6. Medicinal applications of cis-platin and related compounds

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.
9. R. Gopalan and V. Ramlingam, Concise Coordination chemistry, Vikas Publishing house Pvt Ltd., 2001.
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 McGrew Hill, New Delhi,1993.
2. R.C Mehrotra and A.Singh, Organometallic Chemistry- A unified Approach, 2nded, 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.

PROGRAM(s): M.Sc.-I	SEMESTER: II
Course: Paper-II	Course Code: (CHEM 509) Course Title:- Organic Chemistry-II

Teaching Scheme					Evaluation Scheme
Lectures (Hours per week)	Practical (Hours per week)	Tutorial (Hours per week)	Credit	Continuous Assessment (CA) (Marks- 50)	Semester End Examination (Marks- 50)
04	NA	–	04	50	50

Learning Objectives:

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.

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.

3. Accomplish a solution to problems encountered in the field of research.

Course Learning Outcomes.

After completing the course students will be able to:

1) Recognise the type of mechanism & intermediates involved in the given organic reaction and to prove mechanism for the reaction.
2) Identify the ways to modify aliphatic and aromatic compounds via Nucleophilc substitution reactions.
3) Predict the mechanism and stereochemistry of important organic reactions.
4) Understand and write the mechanism of rearrangement reactions with stereochemistry and its applications.
5) Understand the HOMO-LUMO concept and it significance in organic chemistry.
6) Understand the basic principle and concepts in UV and IR spectroscopy
7) Understand the basic concepts of ^{1}H, ^{13}C NMR, and mass spectroscopy.
8) Understand how ^{1}H, ^{13}C NMR and Mass spectroscopy are important for the structure determination of organic compounds.

Course Code: (CHEM 509)

Course Title:-Organic Chemistry-II

Unit-I

1.1. Alkylation of Nucleophilic Carbon Intermediates: (7 L)

1.1.1. Generation of carbanion, kinetic and thermodynamic enolate formation, Regioselectivity in enolate formation, alkylation of enolates.

1.1.2. Generation and alkylation of dianion, medium effects in the alkylation of enolates, oxygen versus carbon as the site of alkylation.

1.1.3. Alkylation of aldehydes, ketones, esters, amides and nitriles.

1.1.4. Nitrogen analogs of enols and enolates- Enamines and Imines anions, alkylation of enamines and imines.

1.1.5. Alkylation of carbon nucleophiles by conjugate addition (Michael reaction).

1.2. Reaction of carbon nucleophiles with carbonyl groups: (8 L)

1.2.1. Mechanism of Acid and base catalyzed Aldol condensation, Mixed Aldol condensation with aromatic aldehydes, regiochemistry in mixed reactions of aliphatic aldehydes and ketones, intramolecular Aldol reaction and Robinson annulation.

1.2.2. Addition reactions with amines and iminium ions; Mannich reaction.

1.2.3. Amine catalyzed condensation reaction: Knoevenagel reaction.

1.2.4. Acylation of carbanions.

Unit-II

2.1. Introduction to Molecular Orbital Theory for Organic Chemistry: (7L)

2.1.1. Molecular orbitals: Formation of σ- and π-MOs by using LCAO method. Formation of π MOs of ethylene, butadiene, 1, 3, 5-hexatriene, allyl cation, anion and radical. Concept of nodal planes and energies of π-MOs

2.1.2. Introduction to FMOs: HOMO and LUMO and significance of HOMO-LUMO gap in absorption spectra as well as chemical reactions. MOs of formaldehyde: The effect of electronegativity perturbation and orbital polarization in formaldehyde. HOMO and LUMO (π and π* orbitals) of formaldehyde.A brief description of MOs of nucleophiles and electrophiles.Concept of 'donor-acceptor' interactions in nucleophilic addition reactions on formaldehyde.Connection of this HOMO-LUMO interaction with 'curved arrows' used in reaction mechanisms.The concept of hardness and softness and its application to electrophiles and nucleophiles.Examples of hard and soft nucleophiles/ electrophiles.Identification of hard and soft reactive sites on the basis of MOs.

2.1.3. Application of FMO concepts in (a) S_N2 reaction, (b) Lewis acid base adducts (BF_3-NH_3 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.

2.2. Applications of UV and IR spectroscopy: (8L)

2.2.1. Ultraviolet spectroscopy: Recapitulation, UV spectra of dienes, conjugated polyenes (cyclic and acyclic), carbonyl and unsaturated carbonyl compounds, substituted aromatic compounds. Factors affecting the position and intensity of UV bands – effect of conjugation, steric factor, pH, and solvent polarity. Calculation of absorption maxima for above classes of compounds by Woodward-Fieser rules (using Woodward-Fieser tables for values for substituents).

2.2.2. Infrared spectroscopy: Fundamental, overtone and combination bands, vibrational coupling, factors affecting vibrational frequency (atomic weight, conjugation, ring size, solvent and hydrogen bonding). Characteristic vibrational frequencies for alkanes, alkenes, alkynes, aromatics, alcohols, ethers, phenols, amines, nitriles and nitro compounds. Detailed study of vibrational frequencies of carbonyl compounds, aldehydes, ketones, esters, amides, acids, acid halides, anhydrides, lactones, lactams and conjugated carbonyl compounds.

Unit III

Reactions and Rearrangements: (15L)

Mechanisms, stereochemistry (if applicable) and applications of the following:

3.1. Reactions: Baylis-Hillman reaction, McMurry Coupling, Corey-Fuchs reaction, Nef reaction, Passerini reaction.

3.2. Concerted rearrangements: Hofmann, Curtius, Lossen, Schmidt, Wolff, Boulton-Katritzky.

3.3. Cationic rearrangements: Tiffeneau-Demjanov, Pummerer, Dienone-phenol, Rupe, Wagner-Meerwein.

3.4. Anionic rearrangements: Brook, Neber, Von Richter, Wittig, Gabriel–Colman, Baker-Venkataraman.

Unit-IV

^{1}H and ^{13}C NMR spectroscopy and Mass spectrometry (15L)

4.1. Proton magnetic resonance spectroscopy: 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,Karplusequation, long range coupling (allylic and aromatic).

4.2. ^{13}C NMR spectroscopy: Theory and comparison with proton NMR, proton coupled and decoupled spectra, off-resonance decoupling. Factors influencing carbon shifts, correlation of chemical shifts of aliphatic, olefin, alkyne, aromatic and carbonyl carbons.

4.3. Mass spectrometry: 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.

4.4. Structure determination involving individual or combined use of the above spectral techniques.

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.Boydand S.K.Bhattacharjee, Pearson Publication (7^{th}Edition)
5. Advanced Organic Chemistry: Reactions and mechanism, B.Millerand R.Prasad, Pearson Education.
6. Advanced Organic Chemistry: Reaction mechanisms, R.Bruckner,AcademicPress.
7. Understanding Organic Reaction Mechanisms, AdamsJacobs, Cambridge University Press.
8. Writing Reaction Mechanism in organic chemistry A. Miller, P. H. Solomons, Academic Press.
9. Principles of Organic Synthesis, R.O.C. Norman and J.M Coxon, NelsonThornes.
10. Advanced Organic Chemistry:Reactions and mechanism, L.G.Wade,Jr.,Maya Shankar Singh, Pearson Education.
11. Mechanism in OrganicChemistry, eter Sykes,6^{th}
12. Molecular OrbitalandOrganic chemical reactions, Ian Fleming Reference Edition, Wiley
13. Introduction to Spectroscopy, DonaldL.Pavia, GaryM.Lampman, GeorgeS.Kriz, Thomson Brooks.
14. Spectrometric Identification of Organic Compounds, R.Silverstein, G.C Basslerand T.C.Morrill, John Wiley and Sons.
15. Organic Spectroscopy,WilliamKemp,W.H.Freeman&Company.
16. Organic Spectroscopy-PrinciplesandApplications,Jagmohan,NarosaPublication.
17. Organic Spectroscopy,V.R.Dani,TataMcGrawHillPublishingCo.
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
21. Organic Reaction Mechanisms, V.K. Ahluwalia, R.K Parasher, Alpha Science International, 2011.
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)

PROGRAM(s): M.Sc.-I		SEMESTER: II			
Course: Paper-III		Course Code: (CHEM 510) Course Title:- Analytical Chemistry-II			
Teaching Scheme					Evaluation Scheme
Lectures (Hours per week)	Practical (Hours per week)	Tutorial (Hours per week)	Credit	Continuous Assessment (CA) (Marks- 50)	Semester End Examination (Marks- 50)
04	NA	–	04	50	50

Course Objectives:

1. To gain knowledge of the chromatography techniques and its applications.
2. To understand application of X-ray spectroscopy for qualitative and quantitative analysis.
3. To introduce radio analytical techniques.
4. To apply the surface analytical techniques for system.
5. To study advantages and applications of electroanalytical methods.

Course outcomes: -

After completion of this Course, the learner will be

1. able to compare the advantages/disadvantages of SEM, STM and TEM.
2. able to develop different techniques to separate the components of mixture.
3. conversant with basic principles and theories of mass spectrometry.
4. able to apply the electroanalytical methods to sample under consideration.
5. able to elaborate on electrogravimetry and coulometry techniques.

Course Code: (CHEM 510)

Course Title :- Analytical Chemistry-II

Unit I -Chromatography [15 L]

1.1 Basic concepts and theories of chromatography: **[5 L]**

- **1.1.1** Introduction and Classification of chromatographic methods.
- **1.1.2** Concept of plate and rate theories in chromatography, efficiency, resolution, selectivity and separation capability.
- **1.1.3** Van Deemter equation and broadening of chromatographic peaks. Optimization of chromatographic conditions**.**

1.2 Gas Chromatography: **[5 L]**

- **1.2.1** Instrumentation –sample injection systems (split/split less), column types (solid/ liquid stationary phases), column switching techniques, temperature programming.
- **1.2.2** Requirements of an ideal detector and types of detectors in GLC and GSC.
- **1.2.3** Applications -Qualitative and quantitative analysis**.**

1.3 High Performance Liquid Chromatography (HPLC):[5 L]

- **1.3.1** Normal phase and reversed phase with special reference to types of commercially available columns (Use of C8 and C18 columns).
- **1.3.2** Diode array type and fluorescence detector.
- **1.3.3** Applications of HPLC.

Unit II - Instrumental methods - II [15L]

2.1 X-ray spectroscopy: **[6 L]**

Principle, instrumentation, applications, advantages and limitations of

- **2.1.1** X-ray absorption spectroscopy. (XAS)
- **2.1.2** X-ray fluorescence spectroscopy (XRF)
- **2.1.3** X-ray diffraction spectroscopy. (XRD)

2.2 Mass spectrometry: **[6 L]**

2.2.1 Instrumentation -

i) Ion sources - electron impact, field ionization, field absorption, chemical ionization and fast atom bombardment sources.
ii) Mass analyzers: Quadrupole, time of flight and ion trap.

2.2.2 Applications

2.3 Radio analytical Methods –[3 L]

2.3.1 Neutron Activation Analysis(NAA)- Introduction, Principle, Theory and Applications.

2.3.2 Advantages and Limitations of NAA.

Unit III- Instrumental methods - III [15L]

3.1 Surface Analytical Techniques – [9 L]

Principle, Instrumentation and Applications of:

3.1.1 Scanning Electron Microscopy (SEM)

3.1.2 Scanning Tunneling Microscopy (STM)

3.1.3 Transmission Electron Microscopy (TEM)

3.2 Atomic Spectroscopy [6 L]

3.2.1 Atomic Spectroscopy based on plasma sources – Introduction, Principle, Instrumentation and Applications.

3.2.2 Advantages and Limitations of AAS

Unit IV -Electroanalytical Methods [15L]

4.1 Ion selective potentiometry and Polarography: [10 L]

(Numericals are Expected)

4.1.1 Ion selective electrodes: Applications of - solid state, precipitate, liquid – liquid, enzyme, gas sensing, bio-catalytic membrane and enzyme-based biosensors electrodes.

4.1.2 Polarography**:** Ilkovic equation, Cottrell equation, effect of complex formation on the polarographic waves.

4.2 Electrogravimetry: **[2 L]**

4.2.1 Introduction, Principle and Instrumentation.

4.2.2 Factors affecting the nature of the deposit.

4.2.3 Applications**.**

4.3 Coulometry: [3 L]

4.3.1 Introduction, Principle and Instrumentation.

4.3.2 Coulometry at controlled potential and controlled current.

References:

Unit I

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

Unit II

1. Essentials of Nuclear Chemistry; H J Arnikar, New Age Publishers (2005)
2. Fundamentals of Radiochemistry; D. D. Sood A. V. R. Reddy and N. Ramamoorthy, , IANCAS 4th edition, 2010
3. Principles of Instrumental Analysis - Skoog, Holler and Nieman, 5th 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, 5th Edition, 1998. Chapters - 23, 24, 25.
2. Analytical Chemistry Principles – ; John H Kennnedy, 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

PROGRAM(s): M.Sc.-I		SEMESTER: II			
Course: Practical		Course Code: PRCHEMOA 511 Course Title:- Chemistry Practical-I (Organic Chemistry and Analytical Chemistry)			
Teaching Scheme				Evaluation Scheme	
Lectures (Hours per week)	Practical (Hours per week)	Tutorial (Hours per week)	Credit	Continuous Assessment (CA) (Marks- 50)	Semester End Examination (Marks- 50)
NA	04	NA	02	50	50

Learning points:

1. To learn Organic mixture separations, purification methods and characterisation steps of organic compounds.
2. To gain knowledge and hands on experience in instrumental and non-instrumental analysis.
3. To introduce the concept of simultaneous determination in spectrophotometry.
4. To study technique of ion exchange and breakthrough capacity.
5. To develop scientific temper and research-based skills.

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

1. learn determination of chemical types of different organic binary mixture
2. learn to separate solid organic binary mixtures on the basis of solubility.
3. learn to purify the separated organic compound by recrystallization technique
4. learn charachterization steps of organic compounds
5. handle and get familiar with SOP's of instruments like potentiometer, conductivity meter, colorimeter and spectrophotometer.
6. understand the concept of complexometric titrations and factors enhancing selectivity of EDTA as a titrant.
7. apply the theory of FES to fertilizers analysis.
8. develop scientific temperament and research-based skills accomplish to encountered in the field of research

Organic Chemistry Practicals

Course Code: PRCHEMOA 511

Separation of Binary mixture using micro-scale technique

1. Separation of binary mixture using physical and chemical methods.
2. Characterization of one of the components with the help of chemical analysis and confirmation of the structure with the help of derivative preparation and its physical constant.
3. Purification and determination of mass and physical constant of the second component.

The following types are expected:

(i) Water soluble/water insoluble solid and water insoluble solid,
(ii) Non-volatile liquid-Non-volatile liquid (chemical separation)
(iii)Water-insoluble solid-Non-volatile liquid.

(Minimum two mixtures from each type and a total of eight mixtures are expected.)

Analytical Chemistry Practicals

Instrumental Experiments

1. To determine the amount of Fe(II) and Fe(III) in a mixture using 1,10-phenanthroline spectrophotometrically.
2. Simultaneous determination of Cr(VI) and Mn(VII) in a mixture spectrophotometrically.
3. To determine the percentage composition of HCl and H_2SO_4 on weight basis in a mixture of two by conductometric titration with NaOH and $BaCl_2$.
4. To determine amount of potassium in the given sample of fertilizers using flame photometer by standard addition method.

Non-Instrumental Experiments

5. To determine the lead and tin content of a solder alloy by titration with EDTA.
6. To determine amount of Cu(II) present in the given solution containing a mixture of Cu(II) and Fe(II).
7. To determine the break through capacity of a cation exchange resin.
8. Estimation of a mixture of Hydrochloric acid and boric acid by acid base titration.

References

1. Quantitative Inorganic Analysis including Elementary Instrumental Analysis by ; A. I. Vogels, 3rd Ed. ELBS (1964)
2. Vogel's textbook of quantitative chemical analysis, Mendham, Denny, Barnes, Thomas, Pearson education, Sixth Ed.
3. Standard methods of chemical analysis ; F. J. Welcher, 1975
4. Standard methods of chemical analysis :Instrumental methods of Analysis ; F. J. Welcher , vol. 3, 1966
5. "Standard methods of Chemical Analysis"; W. W. Scott, Vol. I, Van Nostrand Company, Inc.,1939.
6.,"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 50711)
Course Title:- Physical Chemistry Elective- I

PROGRAM(s): M.Sc.-I		**SEMESTER: II**			
Course: Elective:I		**Course Code: (CHEM50711)** **Course Title:- Physical Chemistry-I**			
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**	**50**	**50**

Learning Objectives:

1.To gain knowledge of the advanced concepts in quantum mechanics, applications of HMO theory, chemical kinetics and molecular dynamics.
2.To understand the advanced concepts in chemical thermodynamics and photochemistry.
3.To develop the skill to solve the problems encountered in the field of quantum and electrochemistry.

Course outcomes

1.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.

2. To understand the use of Schrodinger wave equation in one and two electron systems along with applications of HMO.

3.To develop the skill to solve the problems based on chemical thermodynamics, molecular dynamics and quantum Chemistry.

4.To apply the concept of Jabolonski mechanism in photochemical reactions.

Elective: I Physical Chemistry-I

Unit IQuantum Chemistry II [15 L]

1.1 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.

1.2.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.

1.3.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.

1.4.Hückel Molecular Orbitals theory for ethylene, 1,3-butadiene, cyclobutadiene and benzene. ***(Derivation expected)*** [Ref 7, 8 and 9]

Unit: II Photochemistry 15 L

2.1 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.

2.2Photo 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.

2.3. 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.

(Ref: 17 and 18)

References

1. Peter Atkins and Julio de Paula, Atkin‟s*Physical Chemistry*, 7thEdn., Oxford University Press, 2002.
2. K.J. Laidler and J.H. Meiser, *Physical Chemistry*, 2nd Ed., CBS Publishers and Distributors, New Delhi, 1999.
3. Robert J. Silby and Robert A. Alberty, *Physical Chemistry*, 3rdEdn., John Wiley and Sons (Asia) Pte. Ltd., 2002.
4. Ira R. Levine, *Physical Chemistry*, 5thEdn., Tata McGraw-Hill New Delhi, 2002.
5. G.W. Castellan, *Physical Chemistry*, 3rdEdn.,Narosa Publishing House, New Delhi, 1983.
6. S. Glasstone, *Text Book of Physical Chemistry*, 2ndEdn., McMillan and Co. Ltd., London, 1962.
7. Principles of Chemical Kinetics, 2nd 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, *QuantumChemistry*, 2ndEdn., 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*, 5thEdn., Pearson Education (Singapore) Pte. Ltd., Indian Branch, New Delhi, 2000.
15. Thomas Engel and Philip Reid, Physical Chemistry, 3rdEdn., Pearson Education Limited 2013.
16. D.N. Bajpai, Advanced Physical Chemistry, S. Chand 1stEdn., 1992.
17. C. H. DePuy, O. L. Chapman, Molecular reactions and photoChemistry, Prenticehall of India PVT.LTD.1988.
18. K. K. Rohatgi-Mukherjee. Fundamentals of Photochemistry. Reprint 2002. New Age International Publisher, 1978.
19. Principles of physical Chemistry , Marrown and Prutton 5th edition
20. Essentials of Physical Chemistry ,ArunBahl, B. S Bahl, G. D.Tulli , S Chand and Co. Ltd , 2012 Edition.
21. Introduction of Solids L.V Azaroff , Tata McGraw Hill .
22. Dr. Harichandra A Parbat and Dr. Damodar V Prabhu, Essence of Chemical Kinetics, Sara Publication, First Edition, Sept. 2022.
23. A Text book of physical Chemistry ; Applications of thermodynamics vol III, Mac Millan Publishers India Ltd, 2011
24. New directions in solid state Chemistry, C.N.R. Rao and J Gopalkrishnan , Cambridge University Press.

Elective Practical I

PROGRAM(s): M.Sc.-I	SEMESTER: I				
Course: Practical	Course Code: CHEM50711 Course Title:- Physical and Inorganic Chemistry Practical-I				
TeachingScheme					EvaluationScheme
Lectures(Hoursper week)	Practical(Hoursper week)	Tutorial(Hoursper week)	Credit	ContinuousAssessment(CA)	Semester EndExamination
02	NA	–	02	25	25

Learning Objectives:

Physical Chemistry

1.To gainknowledge 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.

Inorganic Chemistry

1. The learners will be able to synthesize and characterize different inorganic coordination complexes.
2. The learners will be trained in calculating the equilibrium constant for Fe3-/SCN1- by slope intercept method and in determining the electrolytic nature of some inorganic compounds by conductance measurements.

Course Outcomes:-

1.To use the concept of quantum chemistry to interprete the shape and information about the orbitals like 1s, 2pz and 3dz2.

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.

Inorganic Chemistry

1. The learners will characterize different coordination compounds with the help of conductivity measurements, electronic and magnetic measurements and spectroscopic measurements**.**
2. Able to calculating the equilibrium constant for Fe3-/SCN1- by slope intercept method
3. Able to determine the electrolytic nature of some inorganic compounds by conductance measurements.

Elective Chemistry Practical-I

Course Code: CHEM 50711

Physical Chemistry

Non – instrumental:

1.Polar plots of atomic orbitals such as 1*s*, 2Pz and 3*dz2* 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 dialtometric method.

Instrumental:

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 Hammette constant of *m*- and *p*- 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.

References

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

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

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

Elective Chemistry Practical-I

Course Code: CHEM 50711

Inorganic Chemistry

Inorganic Preparations (Synthesis and Characterization)

1) Bis-(tetramethylammonium) tetrachloroCuprate (II) $(Me_4\ N)_2[CuCl_4]$

2) Bis-(tetramethylammonium) tetrachloroNickelate (II) $(Me_4\ N)_2\ [NiCl_4]$

3) Bis (ethylenediammine) Copper (II) Sulphate $[Cu(en)_2]SO_4$

4) HexaaamineNi(II) Sulfate $[Ni(NH_3)_6]SO_4$

5)Potassiumtrioxalato Chromate(III) $K_3[Cr(C_2O_4)_3]$

6) Tetramminemonocarbanato Cobalt (III) Nitrate $[Co(NH_3)_4CO_3]NO_3$

Instrumentation

1) Determination of equilibrium constant by Slope intercept method for Fe^{+3}/ SCN^- system

2) Determination of Electrolytic nature of inorganic compounds by Conductance measurement.

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

Elective: II Physical Chemistry-II

PROGRAM(s): M.Sc.-I		SEMESTER: II			
Course: Elective:II		Course Code: (CHEM50712) 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	50	50

Learning Objectives:

1.To gain knowledge of the advanced concepts in quantum mechanics, applications of HMO theory, chemical kinetics and molecular dynamics.
2.To understand the advanced concepts in chemical thermodynamics and photochemistry.
3.To develop the skill to solve the problems encountered in the field of quantum and electrochemistry.

Course outcomes:-

1.To develop the skill to solve the problems based on molecular dynamics and quantum Chemistry.

2. Learners will able to distinguish between competitive, Noncompetitive and Uncompetitive Inhibition in enzyme-catalysed reactions.

3.Learners will get knowledge of advanced chemical kinetics and molecular dynamics.

4.Leathers will able to use advanced concepts of chemical thermodynamics in chemical reactions.

Course Code: (CHEM50712)

Elective:II Physical Chemistry-II

Unit I

Chemical Thermodynamics II [15 L]

1.1.Fugacity of real gases, Determination of fugacity of real gases using graphical method and from equation of state. Equilibrium constant for real gases in terms of fugacity.Gibbs energy of mixing, entropy and enthalpy of mixing.

1.2.**Real solutions:** Chemical potential in non ideal solutions excess functions of non ideal solutions calculation of partial molar volume and partial molar enthalpy, Gibbs DuhemMargules equation.

1.3.**Thermodynamics of surfaces**, Pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, BET isotherm (derivations expected).

1.4.Bioenergetics : standard free energy change in biochemical reactions, exergonic, endergonic. Hydrolysis of ATP, synthesis of ATP from ADP.

[Ref 2 and 1,10,11,12]

Unit II

Chemical Kinetics and Molecular Reaction Dynamics-II [15 L]

2.1.**Elementary Reactions in Solution:-**Solvent Effects on reaction rates, Reactions between ions- influence of solvent Dielectric constant, influence of ionic strength, Linear free energy relationships Enzyme action

2.2.Kinetics of reactions catalyzed by enzymes -Michaelis-Menten analysis, Lineweaver-Burk and Eadie Analyses**.**

2.3.**Inhibition of Enzyme action**: Competitive, Noncompetitive and Uncompetitive Inhibition. Effect of pH, Enzyme activation by metal ions, Regulatory enzymes.

2.4.**Kinetics of reactions in the Solid State:-**Factors affecting reactions in solids **Rate laws for reactions in solid**: The parabolic rate law, The first order rate Law, the contracting sphere rate law,Contracting area rate law, some examples of kinetic studies.

(Ref: 7 and 2, 22)

References

1. Peter Atkins and Julio de Paula, Atkin‟s*Physical Chemistry*, 7thEdn., Oxford University Press, 2002.
2. K.J. Laidler and J.H. Meiser, *Physical Chemistry*, 2nd Ed., CBS Publishers and Distributors, New Delhi, 1999.
3. Robert J. Silby and Robert A. Alberty, *Physical Chemistry*, 3rdEdn., John Wiley and Sons (Asia) Pte. Ltd., 2002.
4. Ira R. Levine, *Physical Chemistry*, 5thEdn., Tata McGraw-Hill New Delhi, 2002.
5. G.W. Castellan, *Physical Chemistry*, 3rdEdn.,Narosa Publishing House, New Delhi, 1983.
6. S. Glasstone, *Text Book of Physical Chemistry*, 2ndEdn., McMillan and Co. Ltd., London, 1962.
7. Principles of Chemical Kinetics, 2nd Ed., James E. House, ELSEVIER, 2007.
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9. A.K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw – Hill, 1994.
10. R.K. Prasad, *QuantumChemistry*, 2ndEdn., 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.
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15. Thomas Engel and Philip Reid, Physical Chemistry, 3rdEdn., Pearson Education Limited 2013.
16. D.N. Bajpai, Advanced Physical Chemistry, S. Chand 1stEdn., 1992.
17. C. H. DePuy, O. L. Chapman, Molecular reactions and photoChemistry, Prenticehall of India PVT.LTD.1988.
18. K. K. Rohatgi-Mukherjee. Fundamentals of Photochemistry. Reprint 2002. New Age International Publisher, 1978.
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21. Introduction of Solids L.V Azaroff , Tata McGraw Hill .
22. Dr. Harichandra A Parbat and Dr. Damodar V Prabhu, Essence of Chemical Kinetics, Sara Publication, First Edition, Sept. 2022.
23. A Text book of physical Chemistry ; Applications of thermodynamics vol III, Mac Millan Publishers India Ltd, 2011
24. New directions in solid state Chemistry, C.N.R. Rao and J Gopalkrishnan , Cambridge University Press.

Elective Practical II

PROGRAM(s): M.Sc.-I		SEMESTER: I			
Course: Practical		Course Code: CHEM50712 Course Title:- Physical and Inorganic Chemistry Practical-I			
TeachingScheme					EvaluationScheme
Lectures (Hours per week)	Practical (Hours per week)	Tutorial (Hours per week)	Credit	Continuous Assessment (CA)	Semester End Examination
02	NA	–	02	25	25

Learning Objectives:

Physical Chemistry

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.

Inorganic Chemistry

1. The learners will be able to synthesize and characterize different inorganic coordination complexes.
2. The learners will be trained in calculating the equilibrium constant for Fe3-/SCN1- by slope intercept method and in determining the electrolytic nature of some inorganic compounds by conductance measurements.

Course Outcomes:-

1.To use the concept of quantum chemistry to interprete the shape and information about the orbitals like 1s, 2pz and 3dz2.

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.

Inorganic Chemistry

1. The learners will characterize different coordination compounds with the help of conductivity measurements, electronic and magnetic measurements and spectroscopic measurements**.**
2. Able to calculating the equilibrium constant for Fe3-/SCN1- by slope intercept method
3. Able to determine the electrolytic nature of some inorganic compounds by conductance measurements.

Elective Chemistry Practical-I

Course Code: CHEM 50712

Physical Chemistry

Non – instrumental:

1.Polar plots of atomic orbitals such as 1*s*, 2Pz and 3*dz2* 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 dialtometric method.

Instrumental:

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 Hammette constant of *m*- and *p*- 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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1.Practical Physical Chemistry, B. Viswanathan and P.S. Raghavan, Viva Books Private Limited, 2005.

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

Elective Chemistry Practical-I

Course Code: CHEM 50711

Inorganic Chemistry

Inorganic Preparations (Synthesis and Characterization)

1) Bis-(tetramethylammonium) tetrachloroCuprate (II) $(Me_4\ N)_2[CuCl_4]$

2) Bis-(tetramethylammonium) tetrachloroNickelate (II) $(Me_4\ N)_2\ [NiCl_4]$

3) Bis (ethylenediammine) Copper (II) Sulphate $[Cu(en)_2]SO_4$

4) HexaaamineNi(II) Sulfate $[Ni(NH_3)_6]SO_4$

5)Potassiumtrioxalato Chromate(III) $K_3[Cr(C_2O_4)_3]$

6) Tetramminemonocarbanato Cobalt (III) Nitrate $[Co(NH_3)_4CO_3]NO_3$

Instrumentation

1) Determination of equilibrium constant by Slope intercept method for Fe^{+3}/ SCN^- system

2) Determination of Electrolytic nature of inorganic compounds by Conductance measurement.

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

PROGRAM(s): M.Sc-I		SEMESTER: II			
Course:Industrial Training/ Field Projects		Course Code:CHEM512			
Teaching Scheme					Evaluation Scheme
Lectures (Hours per week)	Practical (Hours per week)	Tutorial (Hours per week)	Credit	Continuous Assessment (CA) (Marks-50)	Semester End Examination (Marks- 50)
NA	08	–	04	50	50

Learning Objectives:

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.

Course Outcomes:

At the end of the Course,

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.

PROPOSED MODALITIES 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**

B. External Examination- 50%-

50 Marks per paper Semester End Theory Examination:

1. Duration - These examinations shall be of **two hours** duration.
2. Theory question paper pattern:
   a. There shall be 05 questions each of 10 marks on each unit.
   b. All questions shall be compulsory with internal choice within the questions.

Paper Pattern for 50 marks:

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	

Paper Pattern for 25 marks (Electives):

25 Marks per paper Semester End Theory Examination:

1. Duration - These examinations shall be of **one hour** duration.
2. Theory question paper pattern:

a. There shall be 02 questions each of 08 marks on each unit and one mix question for 09 marks

b. All questions shall be compulsory with internal choice within the questions.

Question	Options	Marks	Questions Based on
Q.1	2 out of 4	08	Unit I
Q.2	2 out of 4	08	Unit II
Q.3	3 out of 6	09	Units (I+II)
	TOTAL	25	

Semester End Practical Examination:

Particulars	Continuous assessment (CA)	Semester end external examination
Laboratory work	15	15
Viva	05	05
Journal	**05**	**05**
Total	**25**	**25**

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.