M.Sc.(2 year) course structure and syllabi
Department of Chemistry,
Central University of Jharkhand, Ranchi

Vision Statement:

The Vision of the Department of Chemistry is the Vision of Central University of Jharkhand, *i.e.*, To develop, enlightened citizenship of a knowledge society for peace and prosperity of individuals, nation and the world, through promotion of innovation, creative endeavors and scholarly inquiry.

Hence, the Department of Chemistry Vision and Mission align with the University vision and the aim of the Department to be the source of knowledge and center of training that imparts a sound foundation in chemical sciences with strong inter and trans-disciplinary academics and research imparting originality and innovation in contemporary and futuristic chemical themes in the line of implementation of National Education Policy – 2020.

Mission Statements (MS) of the Department:

MS1: Providing quality chemical sciences education at all levels including M.Sc., Integrated M.Sc., and doctoral levels
MS2: Conducting fundamental and advanced research in chemical sciences.
MS3: Establishing research collaborations with other universities/institutes/laboratories
MS4: Carrying out sponsored research and development projects (international/national/Government and private partners).

Introduction to the 2 year Master Programme in Chemistry:

The M.Sc. Chemistry programme is prepared for a two year postgraduate studies. The course emphasizes upon the LOCF/CBCS model guides based on the consultation documents on curriculum framework of University Grants Commission and MOOCs. The course includes following attributes in subject such as disciplinary knowledge and skill, critical thinking ability and problem solving, sense of inquiry, ethical awareness and reasoning and finally a momentum on propelling the student for life a long learning. The course curriculum is designed to inculcate a habit of learning continuously through use of advanced ICT technique and other available techniques/books/journals for personal academic growth as well as for increasing employability opportunity. The course also well designed to focus on research and project work taking into account the present day needs as well as societal expectations. The two-year M.Sc. programme also lays emphasis on Industrial /Institutional collaboration as a part of academic curriculum. The programme spread over four semesters and the unique features of the programme are the core courses in Organic, Inorganic, Physical Chemistry, Analytical Chemistry in addition to Instrumentation and Computer Applications, Mathematics for Chemists, Materials Chemistry, Biological Chemistry, seminar course, elective courses and project work in the final semester. Each subject content aims to present a curriculum framework, specifying the curriculum aims, learning targets and objectives, and thus providing suggestions regarding curriculum planning, learning and teaching strategies, assessment and resources.

Graduate Attributes (GA)/Qualification Descriptor (QD):

(i). Disciplinary knowledge and skill: understanding of both theoretical and experimental/applied chemistry knowledge in various fields of interest like Analytical Chemistry, Physical Chemistry, Inorganic Chemistry, Organic Chemistry, Material Chemistry, capable of using of advanced instruments and related soft-wares for in-depth characterization of materials/chemical analysis and separation technology.
(ii). Critical thinker and problem solver: develop critical thinking ability by way of solving problems/numerical using chemistry knowledge and concepts which can be helpful for advanced research career in Chemistry and Chemical Education.
(iii). Sense of inquiry: through appropriate questions, planning and reporting experimental investigation.
(iv). Team player: The course curriculum has been designed to provide opportunity to act as team player by contributing in laboratory, field based situation and industry.
(v). Skilled project manager: by acquiring knowledge about chemistry project management, writing, planning, study of ethical standards and rules and regulations pertaining to scientific project operation.
(vii). Advanced Digitally literate: The course curriculum has been so designed to impart a good working knowledge in understanding and carrying out data analysis, use of library search tools, and use of chemical simulation software and related computational work.
(vii). Ethical awareness/reasoning: to understand and develop ethical awareness/reasoning which the course curriculum adequately provide.
(viii). Lifelong learner: The course curriculum is designed to inculcate a habit of learning continuously through use of advanced ICT technique and other available techniques/books/journals.

Qualification Descriptor (QD) for utilizing basic knowledge and laboratory skills gained in chemical sciences to:

QD1. Analyze, interpret and explain chemically relevant observations
QD2. Identify critical scientific issues and provide potential resolutions
QD3. Create/cultivate new generations of human resource in chemical sciences
QD4. Formulate innovative and relevant chemical problems and develop solutions

Programme Learning Outcome:

PO-1: To formulate new ideas/concepts in chemical sciences.
PO-2: To Analysis and interpretation of chemical phenomena and process.
PO-3: To Design and develop of new molecules/processes with research, industry and societal applications.
PO-4: To acquire the principles and practice of chemical sciences for fundamental research in chemistry and applied chemistry.
PO-5: To get aware about issues of environment, health and development from a chemical perspective and hence to address it using chemistry knowledge.
PO-6: To follow professional ethics in academics and research and in all sphere of life.
PO-7: To develop a leadership quality to work in diverse teams/groups to achieve the goal.
PO-8: To become independent thinker and hence to learn chemistry in the context of scientific advancement and career goal.

Mapping:

	MS1	**MS2**	**MS3**	**MS4**
QD1	√/2	√/3	√/1	√/4
QD2	**√4**	**√/2**	**√/1**	**√/3**
QD3	**√/3**	**√/2**	**√/1**	**√/4**
QD4	**√/1**	**√/4**	**√/3**	**√/2**

Admission and Selection to the Programme:

Through Entrance examination as notified from University from time to time.

Course curriculum Frame work and Syllabi:

M.Sc. (2023 – 2025 batch)

SEMESTER-I				
Sl no	**Subject Code**	**Subject**	**Contact Hours per week (L+T+P)**	**Credits**
1	CHM 610010	Quantum Chemistry	3+1	4
2	CHM 610020	Organic Reactions and Mechanism	3+1	4
3	CHM 610030	Concepts in Coordination Chemistry	3+1	4
4	CHM 611040	Organic Spectroscopy	3+1	4
5	CHM 610050	Organic Chemistry Laboratory I	4	4
6	CHM 610060	Research Methodology	2	2
TOTAL CREDITS				**22**

SEMESTER-II				
Sl no	**Subject Code**	**Subject**	**Contact Hours per week (L+T+P)**	**Credits**
1	CHM 621010	Kinetics and Thermodynamics	3+1	4
2	CHM 621020	Organic Photochemistry and Pericyclic Reactions	3+1	4
3	CHM 621030	Bioinorganic Chemistry	3+1	4
4	CHM 621040	Analytical Chemistry	3+1	4
5	CHM 622060	Physical Chemistry Laboratory	4	4
6	CHM 623060	Seminar	2	2
TOTAL CREDITS				**22**

Course Code: CHM 610010
Title of the Course: Quantum Chemistry
L-T-P: L-3/T-1/P-0

***Course Learning Objectives (CO)*:** This course is intended to introduce students to the quantum chemistry, approximation methods and structure and bonding.
***Course Learning Outcomes (CLO)*:** After the completion of the course, the students will have a comprehensive understanding of the development of scientific ideas about structure and bonding

CLO-1: To develop fundamental understanding of structure and bonding in chemistry on the basis of theory of molecular quantum chemistry aid in deriving quantitative information on structure and properties.
CLO-2: To learn practical tools (combining with theory) to solve Hartree-Fock Equation and density functional theory equation.
CLO-4: To learn improvement of basic method with various electron correlation methods.
CLO-4 : To carry out hand-on exercise to do quantum chemistry calculations with the state-of-the-art software.

Mapping:

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**
CLO1	√/2	√/3	√/1	√/4	**√4**	**√/2**	**√/3**	**√/2**
CLO2	**√/1**	**√/4**	**√/2**	**√/3**	**√/2**	**√/1**	**√/4**	√/1
CLO3	**√/3**	**√/2**	**√/1**	**√/4**	**√/2**	**√/1**	√/2	√/3
CLO4	**√4**	**√/2**	**√/3**	**√/2**	**√/3**	**√/2**	√/3	√/1

UNIT-I: Quantum Chemistry: The Schrodinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrodinger equation to some model systems viz. particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.

UNIT-II: Approximation Methods: The Helium atom. The variation theorem, linear variation principle, Perturbation theory (first order and non-degenerate). Applications of variation method and perturbation theory to the Helium atom.

UNIT-III: Electronic Structure of Atoms: Multielectron atom. Electronic configuration. Russell-Saunders terms and coupling schemes, magnetic effects: spin-orbit coupling and Zeeman splitting.

UNIT-IV Molecular Orbital Theory: H_2+ and H_2 molecules: Valance bond theory (VBT) and molecular orbital theory (MOT) approaches. Homonuclear and Heteronuclear diatoms. Huckel theory of conjugated systems, bond order and charge density calculation. Applications to ethylene, butadiene, cyclopropenyl radical, and cyclobutadiene.

Text books and References:

1. Quantum Chemistry, I. N. Levine, PHI Learning Private Limited.
2. Essentials of Computational Chemistry- Theories and Models, C. J. Cramer, John Wiley and Sons, Ltd.
3. Introduction to Computational Chemistry, F. Jensen, John Wiley and Sons, Ltd.

4. Computational Chemistry- a Practical Guide for Applying Techniques to Real-World Problems, D. C. Young, John Wiley and Sons, Ltd.
Quantum Chemistry, H. Eyring, J. Walter and G. E. Kimball, John Wiley & Sons.
5. Quantum Chemistry, D. A. McQuarrie, University Science Books.
6. Molecular Quantum Mechanics. P. W. Atkins and R. S. Friedman, Oxford University Press.
7. The Chemical Bond, J. N. Murrell, S. F. A. Kettle and J. M. Tedder, John Wiley and Sons.

Course Code: CHM /610020
Title of the Course: Organic Reactions and Mechanisms
L-T-P: L-3/T-1/P-0

***Course Learning Objectives (CO)*:** The learning objective of this paper is to introduce the students to various advanced reactions, reaction mechanisms and dynamics.

***Course Learning Outcomes (CLO)*:** The outcome of the course focused upon developing a
CLO1: critical understanding of reaction mechanism, kinetics and thermodynamics of organic reactions.
CLO2: The student shall be able to understand the methods of formation, structure determination and reactions of the following reactive intermediates: carbocations, carbanions, free radicals, carbenes and nitrenes, arynes and related, species.
CLO3: Detailed reaction mechanisms and effect of different parameters in the regio-, stereo-, chemoselective outcome of addition, substitution, elimination, oxidation, reduction, rearrangement reactions shall be practiced by the students at the end of the course.
CLO4: To prepare the students to apply the mathematics knowledge in learning and understanding other courses in inorganic chemistry and related subjects.

Mapping:

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**
CLO1	√/1	√/3	√/2	√/4	√4	√/3	√/2	√/1
CLO2	√4	√/2	√/1	√/3	√/2	√/1	√/4	√/1
CLO3	√/2	√/3	√/1	√/4	√/2	√/1	√/2	√/3
CLO4	√/1	√/4	√/3	√/2	√/3	√/2	√/3	√/1

UNIT-I: Reaction Mechanism: Structure and Reactivity: (a) Types of mechanism, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin – Hammett principle. Potential energy diagrams, transition statesand intermediates, methods of determining mechanisms, isotope effects. Hard and soft acids and bases. **(b)** Generation, structure, stability and reactivity of carbocations, carbanions, free radicals. Carbenes and nitrenes. Effect of structure on reactivity: resonance and field effect, steric effect, quantitative treatment. The Hammett equation and linear free energy relationships, substitutent and reaction constants. Taft equation.

UNIT-II: Aliphatic Nucleophilic substitution: The SN2, SN1, mixed SN1 and SN2 and SET mechanisms. The neighbouring group mechanism, neighbouring group participation by σ and π bonds, anchimeric assistance. Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations.

The SN1 mechanism: Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ultrasound, ambident nucleophile, regioselectivity.

UNIT-III: Aromatic Nucleophilic Substitution: The SNAr, Sni benzyne and SRN1 mechanisms. Reactivity-effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser, and Smiles rearrangements.

Aromatic Electrophilic Substitution: The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, Ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeier reaction, Gattermann- Koch reaction.

UNIT–IV:Free Radical Reactions: Types of free radical reactions: Free radical substitution, mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic 7alogenations (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction, free radical rearrangement, Hunsdiecker reaction.

Elimination Reactions: The E2, EI and E1cB mechanisms. Orientationof the double bond. Reactivity: Effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

Text books and References:

1. M. B. Smith and J. March, Advanced Organic Chemistry, 6th edition, Wiley, 2007.

2. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry, Structure and Mechanisms, Part A, 5th Edition, Springer, 2007.
3. Reaction and Mechanism in Organic Chemistry by S.P.Singh and S.M.Mukherjee, Trinity Press
4. Organic Chemistry by M.Laudon, Greenwood Village, Colorado
5. Name Reactions and reagents by B.P.Mundy, M.G.Ellerd and F.G. Favaloro Jr., Wiley Interscience
6. Name Reactions 4th Edition by Jie Jack Lee, Springer.
7. Name Reactions and reagents in Organic Synthesis by B.P.Mundi, M.G.Ellerd, and F.G.Favaloro Jr., Wiley
8. Organic Chemistry By J. Clayden S. Warren and N. Greeves, 2nd Edition, Oxford University Press,2017.
9. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, 1st edition, Oxford University Press, 2001.
10. K. Peter C. Vollhardt and N. E. Schore, Organic Chemistry, W. H. Freeman and Company,1999.
11. Peter Sykes, A Guide Book to Mechanism in Organic Chemistry, 6th edition, Pearson Education.

Course Code: CHM /610030
Title of the Course: Concepts in Coordination Chemistry
L-T-P: L-3/T-1/P-0

***Course Learning Objectives (CO)*:** This paper aims to introduce the students to understand the basics of inorganic and coordination chemistry, to understand and analyse structure-property correlation of coordination compounds, coordination compounds and their electronic properties

***Course Learning Outcomes (CLO)*:** This paper will ensure that the students learn appreciate specialized and advanced topics in inorganic and coordination chemistry.

CLO-1 : To understand the basics of inorganic and coordination chemistry.
CLO-2 : To understand and hence to analyse inorganic reaction pathways using redox reactions.
CLO-3 : To understand and hence to analyse structure-property correlation of coordination compounds.
CLO-4: To gain understanding in electronic properties of the molecules and in-depth knowledge to design new coordination compounds.
CLO-5: To appreciate specialized and advanced topics in inorganic and coordination chemistry.

Mapping

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**

CLO1	√/2	√/3	√/1	√/4	**√4**	**√/2**	**√/3**	**√/2**
CLO2	**√4**	**√/2**	**√/1**	**√/3**	**√/2**	**√/1**	**√/4**	√/1
CLO3	**√/3**	**√/2**	**√/1**	**√/4**	**√/2**	**√/1**	√/2	√/3
CLO4	**√/1**	**√/4**	**√/3**	**√/2**	**√/3**	**√/2**	√/3	√/1
CLO5	**√/1**	**√/3**	**√/2**	**√/1**	√/2	√/3	√/1	**√/4**

Unit-I

VSEPR theory - Enumeration of geometrical and optical isomers. Stereochemistry and Bonding in main group compounds, Walsh diagram (tri molecules), d_z-P_{Π} bonds, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules.

Unit-II Oxidation and Reduction: Use of redox potential data - Nernst equation - Influence of complex formation, precipitation, change of pH and concentration on redox potentials - Analysis of redox cycles - Redox stability in water - Disproportionation/Comproportionation - Frost, Latimer and Pourbaix diagrams..

Unit-III Coordination Chemistry: d-orbital splitting in various fields – Spectroscopic states and term symbols - Hole formalism - Tanabe-Sugano and Orgel diagrams - Derivation of Ligand field parameters (Dq.B) from electronic spectra - Magnetic moments - Orbital contribution, spin-orbit coupling and covalency - Molecular orbitals and energy level diagrams for common symmetries - Bonding involving pi-donor ligands - Back-bonding - f-orbital splitting - Spectral and magnetic properties of f-block elements.

Unit-IV: Inorganic Reaction Mechanisms: Substitution reactions - Dissociative and associative interchange - trans -effect - Linear free energy relations - Rearrangements - Berry pseudo rotation - Electron transfer reactions - Photo-dissociation, -substitution and -redox reactions, Fluxional molecules

Books and References:

1. F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 5th Edn, John Wiley, 1988 2. F.A. Cotton , C. A. Murillo, M. Bochmann and R. N. Grimes, ‘’Advanced Inorganic Chemistry’’, 6^{th} Edn Wiley, 1999).

3. J. E. Huheey, E. A. Keiter, R. L. Keiter, ‘’Inorganic Chemistry: Principles of Structure and Reactivity’’, 4th Edn, Prentice Hall, 1997.

4. G. L. Miessler, D. A. Tarr, ‘’Inorganic Chemistry’’, 3rd Edn, Pearson Education, 2004.

5. G. Wulfsberg, ‘’Inorganic Chemistry’’, University Science Books, 2000.

6. Chemistry of the Elements: N. N. B. Greenwood and A. Earnshow, Pergamon.

7. Comprehensive Coordination Chemistry eds.,- G. Wilkinson, R. D. Gillars and J. A.McCleverty, Pergamon.

(2) C. Housecroft, A. G. Sharpe, ‘’Inorganic Chemistry’’, 3rd Edn/4th Edn (2012) Prentice Hall/Pearson, 2008.

Course Code: CHM/610040
Title of the Course: Organic Spectroscopy
L-T-P: L-3/T-1/P-0

Course Learning Objectives: This course is basically focused on structure determination of organic molecules using spectroscopic method such as ultra violet (UV), infrared (IR), nuclear magnetic resonance (NMR) spectroscopy of 1H and 13C and mass spectroscopy (MS). This course introduces the basic principles of electronic transition, selection rule, molecular vibrations and absorption of electromagnetic radiation. Also nuclear spin and interaction of radiation with nucleus and fundamental principle of NMR spectroscopy is discussed. 2D NMR is also discussed such as COSY, NOESY, DEPT, APT for structure determination.

Course Learning Outcomes: After successful completion of this course students should be able

CLO-1: To understand the basic principles of light-matter interactions and learn quantum mechanical methods to analyze the interactions.
CLO-2: To elucidate the structure and molecular mass of small organic molecules using UV, IR, NMR, MS.
CLO-3: To learn various spectroscopic methods based on the IR, magnetic resonance principles.
CLO-4: To analyze spectroscopic information to obtain structural information of molecules.
CLO-5: To calculate the absorption maxima of conjugated molecules using Woodward rule.

Mapping:

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CLO1	√/2	√/3	√/1	√/4	√**4**	√**/2**	√**/3**	√**/2**
CLO2	√**/1**	√**/4**	√**/2**	√**/3**	√**/2**	√**/1**	√**/4**	√/1
CLO3	√**/3**	√**/2**	√**/1**	√**/4**	√**/2**	√**/1**	√/2	√/3
CLO4	√**4**	√**/2**	√**/3**	√**/2**	√**/3**	√**/2**	√/3	√/1
CLO5	√**/1**	√**/4**	√**/2**	√**/1**	√**/4**	√**/2**	√**/3**	√**/2**

UNIT-I:Ultraviolet and Visible Spectroscopy: Various electronic transitions, Beer Lambert law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes, Fieser-Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds, steric effect in biphenyls.

Unit-II: Infrared spectroscopy: Instrumentation and sample handling, characteristics vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines, Detail study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, amides, acids, anhydrides, lactones, lactams, and conjugated carbonyl compounds), Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance, FTIR, IR of gaseous, solid and materials.

UNIT III: Nuclear Magnetic Resonance Spectroscopy (NMR): General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, mechanism of measurement, chemical shift values and correlation for protons bonded to carbon, first order spectra, virtual coupling, stereochemistry, hindered rotation, Fourier transform technique, nuclear overhauser (NOE). Resonance of other materials. Carbon-13 NMR spectroscopy: General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants. Two-dimension NMR spectroscopy – COSY, NOESY, DEPT, APT and INADEQUATE techniques.

UNIT IV Mass spectrometry: Introduction, ion production, fragmentation, single and multiple bond cleavage, rearrangements, cleavage associated with common functional groups, molecular ion peak, metastable ion peak, Nitrogen rule and interpretation of mass spectra

Problems: Structure elucidation based on spectroscopic data (IR, UV, NMR and Mass).

Text Books and References:

1. Spectroscopy methods in Organic Chemistry, I Flemming & B.H.Williams, T.C. Mornil (4th edition) McGraw Hill Book Company 1987.
2. Spectrometric Identification of Organic compounds by R.M. Silverstein, F.X. Webster,David Kiemle (5th edition) John Wiley & Sons, Inc New York,
3. John R. Dyer, Applications of absorption spectroscopy of organic compounds, PHI, 2012.
4. Spectroscopy of Organic Compounds by P. S. Kalsi,New Age International
5. Absorption Spectroscopy of Organic molecules by V.M.Parikh.Addison-Wesley
6. Introduction to Spectroscopy by D.L.Pavia, G.M.Lampman, G.S.Kriz, J.R.Viviyan, 5th Edition, Cengage Learning
7. UV-Vis spectroscopy by C.N.R.Rao, Butterworths, London.

Organic Chemistry Practical CHM- 610050

CHM 610060: Research Methodology

Semester II

Kinetics and Thermodynamics CHM 621010

***Course Learning Objectives (CO)*: This course is intended to introduce students to the physical chemistry related to kinetics and thermodynamics.**

***Course Learning Outcomes (CLO)*: After the completion of the course, the students will have a comprehensive understanding of the development of scientific ideas about Physical chemistry thus Creating, evaluating, analyzing, applying, understanding and remembering of kinetics and thermodynamics**

Unit-I 15hrs

Chemical Kinetics: Potential energy surfaces. Collision theory of reaction rates, Conventional transition state theory (CTST); CTST as applied to ionic reactions, kinetic salt effects. steady state kinetics. Kinetic and thermodynamic control of reactions. Treatment of unimolecular reactions. dynamics of unimolecular reactions (Lindemann- Hinshelwood and Rice Rampsberger -Kassel Marcus (RRKM) theories of unimolecular reactions). Dynamics chain (hydrogenbromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen-bromine and hydrogen - chlorine reactions) and oscillatory reactions (Belousov- Zhabotinski reaction), homogeneous catalysis, kinetics of enzyme reactions. General features of fast reactions, study of fast reactions by flow methods, relaxation methods, Flash photolysis.

Unit-II 15hrs

Chemical Thermodynamics and Phase Diagram: Phase rule, one and two component systems (solid-solid, solid-liquid, solid-vapor, liquid-liquid, liquid-vapor equilibrium), three component systems (Introduction and example). Ehrenfest classification of phase transitions. Phase diagram for semiconductors.

Unit-III 15hrs

Statistical Thermodynamics: Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging, Canonical, grand canonical and microcanonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers) Partition functions-translational, rotational, vibrational and electronic partition functions, calculation of thermodynamic properties in terms of partition function.

Relevant Practicals/Demonstraions: Determination of Consolute Temperature for Phenol Water system, Determination of Partition Co-efficient of a solute in two different solvents, Determination of free energy and entropy from hydrolysis of ester.

Outcome: The students will get aquainted with the reaction dynamics and thermodynamics involved therein such that they can apply the same to various systems.

Text Book

Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 8th Edition, Oxford University Press (2006)

Recommended books & reference

1. Laidler, K. J. *Chemical Kinetics*, 3rd Edition, Pearson Education India (2003)
2. Houston, P. L. *Chemical Kinetics and Reaction Dynamics*, Dover Publications Inc (2006
3. S. Silbey, R. J., Alberty, R. A., Bawendi, M. G. *Physical Chemistry* 4th Edition, Wiley (2006)
5. McQuarrie, D. A. & Simon, J. D. *Physical Chemistry A Molecular Approach* Viva Books (2015)
6. McQuarie, D. A. *Statistical Mechanics* Viva Student Edition, Viva Books (2015)
7. Chandler, D. *Introduction to Modern Statistical Mechanics* Oxford University Press (1987)
8. Dill, K & Bromberg, S. *Molecular Driving Forces: Statistical Thermodynamics in Biology, Chemistry, Physics, and Nanoscience* 2nd Edition, Garland Science (2010)

Organic Photochemistry and Pericyclic Reactions CHM 621020

***Course Learning Objectives (CO)*: This course is intended to introduce students to photochemistry and pericyclic reactions.**

***Course Learning Outcomes (CLO)*: After the completion of the course, the students will have a comprehensive understanding of the development of scientific ideas about photochemistry and pericyclic reactions thus Creating, evaluating, analyzing, applying, understanding and remembering of photochemistry and pericyclic reaxtions.**

Course learning outcome:

After the completion of the course, the students will have a comprehensive understand of the development of scientific ideas in both thermal and photochemical concerted reactions.

CLO-1. To develop fundamentals of thermal and photochemical process with the formation of various excited state.

CLO-2. To learn various thermal and photochemical process through concerted mechanism.

CLO-3. To learn various photochemical reactions through concerted mechanism.

CLO-4. To analyse synthetic applications with hand on exercise in the laboratory.

Unit I: Aromaticity and Symmetry Controlled Reactions Symmetry properties of MO'S. LCAO-MO theory of simple conjugated polyenes and cyclic polyenes. Aromaticity and antiaromaticity.

Homo, hetero and nonbenzenoid aromatic systems. Aromaticity of annulenes. mesoionic compounds

Unit-II: Pericyclic Reactions, Molecular orbital symmetry, Frontier orbitals of ethylene 1,3 butadiene, 1,3,5, hexatriene and allyl system, classification of pericyclic reactions, Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions- conrotatory and disrotatory motion, 4n, 4n+2 and allyl systems. Cycloadditions – antarafacial and suprafacial addition ,4n and 4n+2 systems, 2+2 addition of ketenes, 1,3, dipolar cycloadditions. Sigmatropic rearrangements- suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3, and 5,5 sigmatropic rearrangements. Ene reaction.

Unit III: Organic Photochemistry & Free Radical Reactions Photochemical processes. Energy transfer, sensitization and quenching. Singlet and triplet states and their reactivity. Photoreactions of carbonyl compounds, enes, dienes, and arenes. Norrish reactions of acyclic ketones. Patterno-Buchi, Barton, photo-Fries and Di-pi-methane rearrangement reactions.

Unit IV: Photoreactions of Vitamin D. Photochemistry of vision and photosynthesis. Singlet oxygen generation and reactions. Applications of photoreactions and their applications for industrial synthesis.

Relevant Practicals/Demonstraions: Reaction of Anthracene with Maleic anhydride, Addition of oxygen

Recommended books and references

Organic reactions and orbital symmetry: T. L. Gilchrist and R. C. Storr, CUP Archive
Pericyclic reactions by S. M. Mukherjee
Pericyclic Reaction-A Text Book, S. Sankararamn, Wiley-VCH, Germany, 2005
Pericylic Reactions, Ian Fleming, Oxford Science Publications, New Delhi, 2011
Organic Photochemistry by J.M.Coxon and B. Halton, Cambridge Text in Chemistry
Orbital Symmetry: A Problem solving approach by R.E.Lehr and A.P. Marchand, Academic Press, New York, 1972.

Bioinorganic Chemistry CHM 621030

***Course Learning Objectives (CO)*: This course is intended to introduce students to the bioinorganic chemistry related to chemical kinetics, phase rule and statistical thermodynamics.**

***Course Learning Outcomes (CLO)*: After the completion of the course, the students will have a comprehensive understanding of the development of scientific ideas about bioinorganic chemistry thus Creating, evaluating, analyzing, applying, understanding and remembering of bioinorganic chemistry**

Unit-I:

Metalloenzymes, Iron enzymes – hemoglobin, myoglobin, Superoxide dismutase, catalase, peroxidase and cytochromes, Cyt-P450, hemocyanine, hemerythrine, non-heme iron enzymes, ferredoxin, Molybdenum oxatransferase. Ferritin, transferrin, and siderophores. Xanthine oxidase. Carbonic anhydrase, nitrate reductase. Vitamin B-12.

Unit II Nitrogen fixation and photosynthesis, biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidence, other nitrogenases model systems photosynthesis, active site of chlorophyll, photosystems.

Unit –III: Biochemical Processes in Living system, Phosphate hydrolysis, nucleotide transfer, DNA-polymerase, phosphate transfer, pyruvate kinase, glucose storage, phosphoglucomutase, phosphate storage in muscle, creatine kinase, NaK pump, ATPase. Metal ions / compounds as drugs, chelation therapy. Anticancer and antiarthritis drugs.

Recommended books and references

1. Principles of Bioinorganic Chemistry, S .J. Lippard and J. M. Berg., University Science Books, 1994.

2. Bioinorganic Chemistry, I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valenting, University Science Books.

3. Inorganic Biochemistry vols I and II ed. G. L.Eichhom, Elsevier

4. Progress in Inorganic Chemistry, Vols 18 and 38 ed J. J. Lippard, Wiley

5. Bioinorganic Chemistry, Asim K. Das, Books and Allied, 2nd Ed (2007).

6. Supramolecular Chemistry, J. W. Steed and J. L. Atwood, Willey, 2nd Ed (2009).

7. Bioorganic, Bioinorganic and Supramolecular Chemistry, P.S. Kalsi, J.P. Kalsi, New Age International, 2nd Ed (2012).

8. Bioinorganic Chemistry: Inorganic elements in the Chemistry of life., An Introduction and Guide—Wolfgang Kaim, Brigille Schwedrski John Wiley and sons, 1994

Analytical Chemistry CHM 621040

***Course Learning Objectives (CO)*: This course is intended to introduce students to analytical chemistry.**

***Course Learning Outcomes (CLO)*: After the completion of the course, the students will have a comprehensive understanding of the development of scientific ideas about analytical chemistry thus Creating, evaluating, analyzing, applying, understanding and remembering of analytical chemistry**

Unit-I: Errors, Statistics and Sampling

Accuracy, Precision, Types of errors – determinate and indeterminate errors, minimization of determinate errors, statistical validation- statistical treatment of finite data (mean, median, average deviation, standard deviation, coefficient of variation and variance), significant figures – computation rules, comparison of results – student’s t-test, F-test, statistical Q test for rejection of a result, confidence limit, regression analysis – method of least squares, correlation coefficient, detection limits.

Unit-II: Chromatographic methods of analysis
Introduction, stationary phase, mobile phase, polarity of solvents, retention time, curve width, column adsorption equilibrium, gravity column chromatography, flash column chromatography, advantages and limitations of column chromatography. Gas Chromatography (GC): Introduction, instrumentation, types of columns (packed, open tubular etc.), types of detectors (TCD, ID, FID, ECD, element selective detectors), applications of GC for quantitative analysis. High performance liquid chromatography (HPLC): Introduction, Instrumentation, Types of liquid chromatography. Applications.
Unit-III: Spectroscopic Methods of Analysis UV-visible spectroscopy, Instrumentation, Calibration, Baseline Correction IR Spectroscopy: Instrumentation, sample handling, Fourier transform infrared spectroscopy Principle, instrumentation & its advantages. Raman Spectroscopy: Theory, Instrumentation, sample handling, Illumination diagnosis and structure analysis, polarization measurements, quantitative analysis. Principles of AAS, Instrumentation – flame AAS and furnace AAS, resonance line sources, sensitivity and detection limits in AAS, interferences –chemical and spectral, evaluation methods in AAS and application in qualitative and quantitative analysis. Atomic Emission Spectroscopy (AES): Principles of AES, Instrumentation, evaluation methods, Application in quantitative analysis.

Relevant Practicals/Demonstraions: Preparation of TLC, Separation using Column Chromatography, Varification of Beer-Lambert’s Law

Recommended books and references:

1. Analytical Chemistry, G. D. Christian, 4 th Ed. John Wiley, New York (1986)
2. Instrumental methods of Analysis, H. H. Willard, L. L. Merritt, Jr J. A. Dean and F. A. Settle Jr 6th Ed CBS (1986).
3. Instrumental Methods of Analysis-G-Chatwal and S. Anand (Himalaya Publication;1988).
4. Introduction to Instrumentation Analysis by R.D. Braun Pharma Med Press.
5. Instrumental methods of chemical Analysis, B.K. Sharma, 16th edition Goel Publishing House.
6. Fundamentals of Analytical Chemistry, D. A. Skoog and D. M. West and F. J. Holler Holt-Saunders 6th Edition (1992).
7. Principles of Instrumental Analysis, D. A. Skoog, F. J. Holler and J.A. Niemann 5th Edition (1998)

Physical Chemistry Laboratory CHM 622060

Error Analysis and Statistical Data Analysis Errors, types of errors, minimization of errors, error distribution curves, precision, accuracy and combination; statistical treatment for error analysis, student ‘t’ test, null hypothesis, rejection criteria, F & Q test; linear regression analysis, curve fitting.

Calibration of volumetric apparatus, burette, pipette and standard flask. Adsorption To study surface tension – concentration relationship for solutions (Gibbs equation)

Chemical Kinetics (i) Determination of the effect of (a) Change of temperature (b) Change of concentration of reactants and catalyst and (c) Ionic strength of the media on the velocity constant of hydrolysis of an ester / ionic reactions.
(ii) Determination of the velocity constant of hydrolysis of an ester / ionic reaction in micellar media.
(iii) Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide studying the kinetics as an iodine clock reaction.
(iv) Determination of the degree of dissociation of weak electrolyte and to study the deviation from ideal behaviour that occurs with a strong electrolyte. Electrochemistry A. Conductometry:
(v) Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide conductometrically.
(vi) Determination of solubility and solubility product of sparingly soluble (e.g., PbSO4, BaSO4) conductometrically.
(vii) Determination of the strength of strong and weak acids in a given mixture conductometrically.
(viii) Determination of the activity coefficient of zinc ions in the solution of 0.002 M zinc sulphate using Debye Huckel's limiting law. B. Potentiometry / pH metry: (i) Determination of strengths of halides in a mixture potentionmetrically.
(ix) Determination of the valency of mercurous ions potentiometerically.
(x) Determination of the strength of strong and weak acids in a given mixture using a potentiometer / pH meter.
(xi) Acid-base titration in a non-aqueous media using a pH meter.
(xii) Determination of the dissociation constant of acetic acid in acetone by titrating it with KOH in what medium.
(xiii) Determine the PK's of a dibasic acid by pH titration using a pH meter.

(xiv) Determination of rate constant for hydrolysis / inversion of sugar using a polarimeter.
(xv) Enzyme kinetics – inversion of sucrose.

Books Recommended

1. Practical Physical Chemistry, A. M. James and F.E. Prichard, Longman.
2. Findley's Practical Physical Chemistry, B. P. Levitt, Longman.
3. Experimental Physical Chemistry, R. C. Das and B. Behera, Tata McGraw Hill, 1983, New Delhi.
4. Vogel's Text book of Quantitative Analysis, revised, J.Bassett, R.C.Denney, G.H. Jeffery and J.Mendham, ELBS.
5. Fundamentals of Analytical Chemistry, D.A.Skoog, D.M.West and F.J.Hollar. 7th Edition, Harcourt College Publishers, 1996.

Seminar CHM 623060

SEMESTER-III				
Sl no	**Subject Code**	**Subject**	**Contact Hours per week (L+T+P)**	**Credits**
1		Organometallic Chemistry	3+1	4
2		Group Theory, Molecular Spectroscopy and Surface Chemistry	3+1	4
3		Main Group Chemistry, Actinides, Lanthanides and Nuclear Chemistry	3+1	4
4		MOOCs I (Organic reaction mechanism)	4	4
5		Inorganic Chemistry laboratory	4	4
6		Minor Project	4	4
TOTAL CREDITS				**24**

SEMESTER-IV				
Sl no	**Subject Code**	**Subject**	**Contact Hours per week (L+T+P)**	**Credits**
1		Major Project		20
2		MOOCs II		4
3				
TOTAL CREDITS				**24**

Organometallic Chemistry

***Course Learning Objectives (CO)*: This course is intended to introduce students to organometallic chemistry.**

***Course Learning Outcomes (CLO)*: After the completion of the course, the students will have a comprehensive understanding of the development of scientific ideas about organometallic chemistry thus Creating, evaluating, analyzing, applying, understanding and remembering of organometallic chemistry**

Self-Study:

Definition, Classes of ligands, haptacity, 18-electron rule and its applications. Metal-alkene, Metal-alkyne complexes, metal-dinitrogen compounds: Zeises salt (preparation, structure and bonding), Sandwich molecules, Ferrocene (preparation, structure and reactions).

Unit-I **15hrs**

Metal Carbonyls and Nitrosyls: Structure, nature of bonding, interpretation using IR spectroscopy, syntheses and reactivity.

Metal-phosphines: Structure, nature of bonding, steric and electronic parameter, basicity of phosphines.

Metal carbenes: Classification (Fischer carbenes and Schrock carbenes), Structure, nature of bonding, syntheses, reactivity and applications.

Tebbe's reagent: preparation and its applications.

N-heterocyclic carbenes: Preparation, bonding nature with transition metals and reactivity. Metal-cyanide, Metal-isocyanides

Unit-II **15hrs**

Study of Organometallic Compounds: Organo-magnesium, Organo-aluminium, Organo-zinc and Organo-lithium, Organo cupper reagents, Corey-House synthesis, Gilman reagents and its applications.

Metathesis: Definition, synthetic tool, synthesis of metathesis catalysts (Grubbs' and Schrock), mechanism of ring opening metathesis (ROM), cross metathesis (CM), ring closing metathesis (RCM), ring opening metathesis polymerization (ROMP) and enyne metathesis (EM). Few applications

Unit-III **15hrs**

Basic organometallic reaction mechanism: Oxidative addition, Reductive elimination, Migratory insertion, Alkene insertion, β-hydride elimination, Transmetallation.

Pd, Cu, Ni cross coupling reactions: The Heck reaction, Suzuki-Miyaura, Sonogashira, Stille, Kumada, Negishi, Hiyama coupling, Buchwald-Hartwig C-N cross coupling, Fukuyama coupling, Chan Lam coupling, Ullmann Reaction, Cadiot-Chodkiewicz Coupling, Glaser Coupling, Eglinton Reaction. Olefin polymerization, Oxo, Wacker processes, Monsanto acetic acid, Ziegler-Natta, ZSM, Catalytic cycle of Wilkinson's catalyst; Iridium/Ruthenium based catalysts for asymmetric hydrogenation.

Recommended books

1. "Organometallic Chemistry of the Transition Metals", R. H. Crabtree, Wiley, New York, 1988.
2. "Organometallics: A Concise Introduction", C. Elschenbroich and A. Salzer, 3rd Edn.1999.
3. "Basic Organometallic Chemistry" B D Gupta, A J Elias, 2nd Edn. 2013, Universities Press

Group Theory, Molecular Spectroscopy and Surface Chemistry

***Course Learning Objectives (CO)*: This course is intended to introduce students to group theory, molecular spectroscopy and surface chemistry.**

***Course Learning Outcomes (CLO)*: After the completion of the course, the students will have a comprehensive understanding of the development of scientific ideas about group theory, molecular spectroscopy and surface chemistry thus Creating, evaluating, analyzing, applying, understanding and remembering of group theory, molecular spectroscopy and surface chemistry**

Unit-I: Group theory:

Symmetry elements and Symmetry operation, Groups and Subgroups, Point group. Schonflies notation, matrix representations of groups, irreducible representations and character tables. The Great Orthogonality theorem and its importance. Derivation of character table. Application of group theory in Quantum Mechanics, Chemical Bonding, Metal Complexes, Spectroscopy

Unit-II: Molecular Spectroscopy:

The rigid diatomic rotor, energy eigenvalues and eigenstates, selection rules, intensity of rotational transitions, the role of rotational level degeneracy, the role of nuclear spin in determining allowed rotational energy levels. Classification of polyatomic rotors and the non-rigid rotor. Vibrational spectroscopy, harmonic and anharmonic oscillators, Morse potential, mechanical and electrical anharmonicity, selection rules. The determination of anharmoncity constant and equilibrium vibrational frequency from fundamental and overtones. Normal modes of vibration, internal and symmetry coordinates. Basics of Raman spectroscopy, Electron Spin Resonance Spectroscopy, Mossbauer Spectroscopy.

Unit-III: Surface Chemistry:

Adsorption, Surface tension, capillary action, pressure difference across curved surface, vapour pressure of droplets. Gibbs adsorption isotherm, estimation of surface area (BET equation), surface films on liquids (Electrokinetic phenomenon), catalytic activity at surfaces. Surface active agents, classification of surface-active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants counter ion binding to micelles, thermodynamics of micellization, phase separation and mass action models, solubilization, micro emulsion, reverse micelles.

Self-Study:

1. Recognizing the significance and utilizing group theory in chemical systems
2. Discern the connection between classical and statistical thermodynamics.
3. Probe into the physical properties of molecules.

Recommended Textbooks / references:

1. Cotton, F. A. Chemical Applications of Group Theory 3rd Edition, Wiley (2008).

2. Carter, R. L. Molecular Symmetry and Group Theory Wiley Student Edition, Wiley (2009).
3. Bishop, D. M. Group Theory and Chemistry Dover Publications Inc (1993)
4. McQuarie, D. A. Statistical Mechanics Viva Student Edition, Viva Books (2015)5. Chandler, D. Introduction to Modern Statistical Mechanics Oxford University Press (1987)
6. Dill, K & Bromberg, S. Molecular Driving Forces: Statistical Thermodynamics in Biology, Chemistry, Physics, and Nanoscience 2nd Edition, Garland Science (2010)
7. Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry 8th Edition, Oxford University Press (2006).
8. Silbey, R. J., Alberty, R. A., Bawendi, M. G. Physical Chemistry 4th Edition, Wiley (2006

Main Group Chemistry, Actinides, Lanthanides and Nuclear Chemistry

***Course Learning Objectives (CO)*: This course is intended to introduce students to main group chemistry.**

***Course Learning Outcomes (CLO)*: After the completion of the course, the students will have a comprehensive understanding of the development of scientific ideas about main group chemistry thus Creating, evaluating, analyzing, applying, understanding and remembering of main group chemistry**

Unit-I: Stereochemistry and Bonding in main group compounds VSEPR, Walsh diagram (tri molecules), dz-Pp bonds, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules. General characteristics, Allotropes, Structure and Reactions of simple and industrially important compounds: Boranes, Carboranes, Silicones, Silicates, Boron nitride, Borazines and Phosphazenes.

Unit-II: General characteristics, Structure and Reactions of simple and industrially important compounds: Hydrides, Halides, Oxides and Oxoacids of pnictogens (N, P), chalcogens (S, Se & Te) and halogens, Xenon compounds, Pseudo halogens and Interhalogen compounds.

Unit-III: Lanthanides, actinides, extraction, separation, purification, application, contractions and its significance, post actinide elements, radioactive elements, half-life, disintegration, radiocarbon dating, tracer techniques, and use in medicinal, agricultural and structural interpretations, nuclear reactions as source of energy.

Relevant Practicals/Demonstraions:

1. Separation of few lanthanides by fractional crystallization, and elution chromatography, determination of Rf.
2. Estimation of halides and pseudo-halides using argentometric titration using indicators.
3. Estimation of nitrate, phosphate, borate, and sulphate in unknown samples.

Recommended books & references*:*

1. Chemical Application of Group Theory: F. A. Cotton, John Wiley.
2. Symmetry in Chemistry: Orchin and Jaffe.
3. Group theory: K. V. Raman, Tata McGraw Hill.
4. Advanced Inorganic Chemistry: F. A. Cotton and G. Wilkinson, John Wiley.
5. Inorganic Chemistry: J.E. Huheey, E. A. Keiter, R. L. Keiter, Pearson Education.
6. Chemistry of the Elements: N. N. B. Greenwood and A. Earnshow, Pergamon
7. Comprehensive Coordination Chemistry eds,- G. Wilkinson, R. D. Gillars and J A. McCleverty, Pergamon.
8. Fundamental concepts of Inorganic Chemistry – A. K. Das (Vol 2), CBS.
9. General and Inorganic Chemistry- Part 2, R. Sarkar, Central pubication
10. Inorganic Chemistry – Wulfsberg, Viva.

MOOCs I (Organic reaction mechanism)

UNIT I
Broad classification of reactions and basics of arrow pushing, Reaction co-ordinate diagrams Reaction Kinetics: rate laws and methods of determining concentration. Introduction to linear free energy relationships, Linear Free Energy Relationships.
UNIT II
Kinetic and equilibrium isotope Effects, Miscellaneous methods to determine mechanisms: isotope labelling, trapping of intermediates, checking for common intermediate, competition and cross-over experiments.
UNIT III
Catalysis: classification and introduction to Bronstead acid catalysis, Types of Catalysis: Acid, Binding, Electrophilic, Nucelophilic, Covalent, Proximity and Phase-transfer

Analytical Chemistry Practical

1. Analysis of Bronze with respect to Copper and Tin
2. Analysis of Dolomite ore for Ca, Mg and Silicate material
3. Analysis of Cement with respect to SiO_2, Calcium, Iron, Magnesium and Aluminium
4. Spectrophotometric determination of lead in leaves using dithizone-chelating agent
5. Determination of alcohol from given sample spectrophotometrically
6. Determination of Nitrogen from Fertilizer sample
7. Determination of Phosphate from fertilizer sample by volumetric method.
8. Removal of dyes on activated charcoal by column chromatography
9. Determination of COD from waste water
10. Analysis of water with respect to sulphate & Chloride
11. Determination of organic carbon in soil

Minor Project (shall be carried out under the supervision of Dept faculty members/joint guidance involving faculty members of other Dept./School/Institute –University of repute as per the procedure of CUJ).

Semester IV

MOOCs II

Major Project

In the final semester (IVth semester), students have to carry out project work at CUJ as per the recommendation of faculty committee of the Department/centre under the supervision of a scientist/Faulty member. Joint collaboration with other Departments/centres/schools is encouraged in order to enhance the quality of work and interdisciplinary characteristics in the work. The Area of the work is to be decided by the Adviser(s). On completion of the Project work, students have to submit their work in the form of a dissertation followed by oral presentation in the presence of Faculty members and an external expert member.

2 Year M.Sc. in Chemistry
Detailed Course Structure
2022 – 2024

SEMESTER-I				
Sl no	**Subject Code**	**Subject**	**Contact Hours per week (L+T+P)**	**Credits**
1	CHM 610010	Quantum Chemistry	3+1	4
2	CHM 610020	Organic Reactions and Mechanism	3+1	4
3	CHM 610030	Concepts in Coordination Chemistry	3+1	4
4	CHM 611040	Organic Spectroscopy	3+1	4
5	CHM 610050	Organic Chemistry Laboratory I	2	2
6	CHM 610060	Inorganic Chemistry Laboratory	2	2
TOTAL CREDITS				**20**

SEMESTER-II				
Sl no	**Subject Code**	**Subject**	**Contact Hours per week (L+T+P)**	**Credits**
1	CHM 621010	Kinetics and Thermodynamics	3+1	4
2	CHM 621020	Organic Photochemistry and Pericyclic Reactions	3+1	4
3	CHM 621030	Bioinorganic Chemistry	3+1	4
4	CHM 621040	Analytical Chemistry	3+1	4
5	CHM 622060	Physical Chemistry Laboratory	2	2
6	CHM 623060	Seminar	2	2
TOTAL CREDITS				**20**

Semester I

Quantum Chemistry CHM 610010

***Course Learning Objectives (CO)*: This course is intended to introduce students to quantum chemistry.**

***Course Learning Outcomes (CLO)*: After the completion of the course, the students will have a comprehensive understanding of the development of scientific ideas about quantum chemistry thus Creating, evaluating, analyzing, applying, understanding and remembering of quantum chemistry**

UNIT-I: Quantum Chemistry: The Schrodinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrodinger equation to some model systems viz. particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.

UNIT-II: Approximation Methods: The Helium atom. The variation theorem, linear variation principle, Perturbation theory (first order and non-degenerate). Applications of variation method and perturbation theory to the Helium atom.

UNIT-III: Electronic Structure of Atoms: Multielectron atom. Electronic configuration. Russell-Saunders terms and coupling schemes, magnetic effects: spin-orbit coupling and Zeeman splitting.

UNIT-IV Molecular Orbital Theory: H2+ and H2 molecules: Valance bond theory (VBT) and molecular orbital theory (MOT) approaches. Homonuclear and Heteronuclear diatoms. Huckel theory of conjugated systems, bond order and charge density calculation. Applications to ethylene, butadiene, cyclopropenyl radical, and cyclobutadiene.

Text books and References:

1. Quantum Chemistry, I. N. Levine, PHI Learning Private Limited.
2. Essentials of Computational Chemistry- Theories and Models, C. J. Cramer, John Wiley and Sons, Ltd.
3. Introduction to Computational Chemistry, F. Jensen, John Wiley and Sons, Ltd.
4. Computational Chemistry- a Practical Guide for Applying Techniques to Real-World Problems, D. C. Young, John Wiley and Sons, Ltd.
5. Quantum Chemistry, H. Eyring, J. Walter and G. E. Kimball, John Wiley & Sons.
6. Quantum Chemistry, D. A. McQuarrie, University Science Books.
7. Molecular Quantum Mechanics. P. W. Atkins and R. S. Friedman, Oxford University Press.
8. The Chemical Bond, J. N. Murrell, S. F. A. Kettle and J. M. Tedder, John Wiley and Sons.

Organic Reactions and Mechanisms CHM 610020

***Course Learning Objectives (CO)*: This course is intended to introduce students to organic reactions and mechanisms.**

***Course Learning Outcomes (CLO)*: After the completion of the course, the students will have a comprehensive understanding of the development of scientific ideas about organic reactions and mechanisms thus Creating, evaluating, analyzing, applying, understanding and remembering of organic reactions and mechanisms**

Course learning outcome:

1. Substitution reaction mechanism, elimination reaction, radical reaction, and stereochemistry.
2. Organic chemistry with emphasis on various examples/name reactions.
3. Substitution reaction mechanism in aromatic systems.
4. Radical reaction mechanism in organic chemistry.

UNIT-I: Reaction Mechanism: Structure and Reactivity: (a) Types of mechanism, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin – Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects. Hard and soft acids and bases. **(b)** Generation, structure, stability and reactivity of carbocations, carbanions, free radicals. Carbenes and nitrenes. Effect of structure on reactivity: resonance and field effect, steric effect, quantitative treatment. The Hammett equation and linear free energy relationships, substitutent and reaction constants. Taft equation.

UNIT-II: Aliphatic Nucleophilic substitution: The SN^2, SN^1, mixed SN^1 and SN^2 and SET mechanisms. The neighbouring group mechanism, neighbouring group participation by σ and π bonds, anchimeric assistance. Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations. The SN^1 mechanism: Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ultrasound, ambident nucleophile, regioselectivity.

UNIT-III: Aromatic Nucleophilic Substitution: The SNAr, Sni benzyne and SRN^1 mechanisms. Reactivity-effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser, and Smiles rearrangements.

Aromatic Electrophilic Substitution: The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, Ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeier reaction, Gattermann- Koch reaction.

UNIT–IV: Free Radical Reactions: Types of free radical reactions: Free radical substitution, mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenations (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction, free radical rearrangement, Hunsdiecker reaction.

Elimination Reactions: The E_2, E_I and E_1cB mechanisms. Orientationof the double bond. Reactivity: Effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

Text books and References:

1. M. B. Smith and J. March, Advanced Organic Chemistry, 6th edition, Wiley, 2007.
2. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry, Structure and Mechanisms, Part A, 5th Edition, Springer, 2007.
3. Reaction and Mechanism in Organic Chemistry by S. P. Singh and S. M. Mukherjee, Trinity Press
4. Organic Chemistry by M.Laudon, Greenwood Village, Colorado
5. Name Reactions and reagents by B.P.Mundy, M.G.Ellerd and F.G. Favaloro Jr., Wiley Interscience
6. Name Reactions 4th Edition by Jie Jack Lee, Springer
7. Name Reactions and reagents in Organic Synthesis by B.P.Mundi, M.G.Ellerd, and F.G.Favaloro Jr., Wiley
8. Organic Chemistry by J. Clayden S. Warren and N. Greeves, 2nd Edition, Oxford University Press, 2017.
9. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, 1st edition, Oxford University Press, 2001.
10. K. Peter C. Vollhardt and N. E. Schore, Organic Chemistry, W. H. Freeman and Company,1999.
11.Peter Sykes, A Guide Book to Mechanism in Organic Chemistry, 6th edition, Pearson Education.

Concepts in Coordination Chemistry   CHM 610030

***Course Learning Objectives (CO)*: This course is intended to introduce students to coordination chemistry.**

***Course Learning Outcomes (CLO)*: After the completion of the course, the students will have a comprehensive understanding of the development of scientific ideas about coordination chemistry thus Creating, evaluating, analyzing, applying, understanding and remembering of coordination chemistry**

Unit-I

VSEPR theory - Enumeration of geometrical and optical isomers. Stereochemistry and Bonding in main group compounds, Walsh diagram (tri molecules), dz-P∏ bonds, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules. **Unit-II** Oxidation and Reduction: Use of redox potential data - Nernst equation - Influence of complex formation, precipitation, change of pH and concentration on redox potentials – Analysis of redox cycles - Redox stability in water - Disproportionation/Comproportionation - Frost, Latimer and Pourbaix diagrams.

Unit-III Coordination Chemistry: d-orbital splitting in various fields – Spectroscopic states and term symbols - Hole formalism - Tanabe-Sugano and Orgel diagrams - Derivation of Ligand field parameters (Dq.B) from electronic spectra – Magnetic moments - Orbital contribution, spin-orbit coupling and covalency - Molecular orbitals and energy level diagrams for common symmetries - Bonding involving pi-donor ligands - Back-bonding - f-orbital splitting – Spectral and magnetic properties of f-block elements.

Unit-IV: Inorganic Reaction Mechanisms: Substitution reactions - Dissociative and associative interchange - trans -effect - Linear free energy relations - Rearrangements - Berry pseudo rotation - Electron transfer reactions - Photo-dissociation, -substitution and -redox reactions, Fluxional molecules

Books and References*:*

1. F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 5th Edn, John Wiley, 1988
2. F.A. Cotton, C. A. Murillo, M. Bochmann and R. N. Grimes, Advanced Inorganic Chemistry, 6th Edn Wiley, 1999).
3. J. E. Huheey, E. A. Keiter, R. L. Keiter, ‘’Inorganic Chemistry: Principles of Structure and Reactivity’’, 4th Edn, Prentice Hall, 1997.
4. G. L. Miessler, D. A. Tarr, ‘’Inorganic Chemistry’’, 3rd Edn, Pearson Education, 2004.
5. G. Wulfsberg, ‘’Inorganic Chemistry’’, University Science Books, 2000.
6. Chemistry of the Elements: N. N. B. Greenwood and A. Earnshow, Pergamon.
7. Comprehensive Coordination Chemistry ed. G. Wilkinson, R. D. Gillars and J. A.McCleverty, Pergamon.
8. C. Housecroft, A. G. Sharpe, ‘’Inorganic Chemistry’’, 3rd Edn/4th Edn (2012) Prentice Hall/Pearson,

Organic Spectroscopy CHM 611040

***Course Learning Objectives (CO)*: This course is intended to introduce students to organic spectroscopy.**

***Course Learning Outcomes (CLO)*: After the completion of the course, the students will have a comprehensive understanding of the development of scientific ideas about organic spectroscopy thus Creating, evaluating, analyzing, applying, understanding and remembering of organic spectroscopy**

UNIT-I: Ultraviolet and Visible Spectroscopy: Various electronic transitions, Beer Lambert law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes, Fieser Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds, steric effect in biphenyls.

Unit-II: Infrared spectroscopy: Instrumentation and sample handling, characteristics vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines, Detail study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, amides, acids, anhydrides, lactones, lactams, and conjugated carbonyl compounds), Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance, FTIR, IR of gaseous, solid and materials.

UNIT III: Nuclear Magnetic Resonance Spectroscopy (NMR): General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, mechanism of measurement, chemical shift values and correlation for protons bonded to carbon, first order spectra, virtual coupling, stereochemistry, hindered rotation, Fourier transform technique, nuclear overhauser (NOE). Resonance of other materials. Carbon-13 NMR spectroscopy: General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants. Two-dimension NMR spectroscopy – COSY, NOESY, DEPT, APT and INADEQUATE techniques.

UNIT IV Mass spectrometry: Introduction, ion production, fragmentation, single and multiple bond cleavage, rearrangements, cleavage associated with common functional groups, molecular ion peak, metastable ion peak, Nitrogen rule and interpretation of mass spectra Problems: Structure elucidation based on spectroscopic data (IR, UV, NMR and Mass).

Text Books and References:

1. Spectroscopy methods in Organic Chemistry, I Flemming & B.H.Williams, T.C. Mornil (4th edition) McGraw Hill Book Company 1987.

2. Spectrometric Identification of Organic compounds by R.M. Silverstein, F.X. Webster, David Kiemle (5th edition) John Wiley & Sons, Inc New York

3. John R. Dyer, Applications of absorption spectroscopy of organic compounds, PHI, 2012.

4. Spectroscopy of Organic Compounds by P. S. Kalsi, New Age International

5. Absorption Spectroscopy of Organic molecules by V. M. Parikh. Addison-Wesley

6. Introduction to Spectroscopy by D. L. Pavia, G. M. Lampman, G. S. Kriz, J. R. Viviyan, 5th Edition, Cengage Learning

7. UV-Vis spectroscopy by C. N. R. Rao, Butterworths, London.

Chemistry Practical-I CHM 610050

1. Synthesis of dibromocinnamic acid, Reaction of dibromo compounds with Zinc, Reaction of epichlorohydrin with amines, Conversion of alcohol to amine through tosylation, Swern Oxidation.

2. Determination of Consolute Temperature for Phenol-Water system, Determination of Partition Co-efficient of a solute in two different solvents, Determination of free energy and entropy from hydrolysis of ester.

3. Separation Techniques: TLC

4. Separation of few lanthanides by fractional crystallization, and elution chromatography, determination of Rf.

5. Estimation of halides and pseudo-halides using argentometric titration using indicators.
6. Estimation of nitrate, phosphate, borate, and sulphate in unknown samples.

Recommended books and references:

1. The Systematic Identification of Organic Compounds: R.L. Shriner, C. K. F. Harmann, T.C.Morrill, D.Y. Curtin, R.C. Fusion, John Wiley and Sons.
2. Organic Analytical Chemistry (Theory and Practice): Jagmohan, Narosa Publishing House.
3. A Text Book of Practical Organic Chemistry: Arthur I.Vogel, .E.L.B.S. and Longman.
4. Experiments and Techniques in Organic Chemistry: D. Pasto, C. Johnson.
5. Laboratory Mannual of Organic Chemistry: B.B. Dey and M.V.Siaram (Revised)-:T.R.Govindachari, Allied Publishers.
6. Systematic Qualitative Organic Analysis: H. Middleton, Orient Longman.
7. A Hand Book of Organic Analysis (Qualitative and Quantitative): H.T. Clarke, Revised, B.Haynes, Arnold Publishers.

Semester II

Kinetics and Thermodynamics CHM 621010

***Course Learning Objectives (CO)*: This course is intended to introduce students to the physical chemistry related to kinetics and thermodynamics.**

***Course Learning Outcomes (CLO)*: After the completion of the course, the students will have a comprehensive understanding of the development of scientific ideas about Physical chemistry thus Creating, evaluating, analyzing, applying, understanding and remembering of kinetics and thermodynamics**

Unit-I

Chemical Kinetics: Potential energy surfaces. Collision theory of reaction rates, Conventional transition state theory (CTST); CTST as applied to ionic reactions, kinetic salt effects. steady state kinetics. Kinetic and thermodynamic control of reactions. Treatment of unimolecular reactions. dynamics of unimolecular reactions (Lindemann- Hinshelwood and Rice Rampsberger -Kassel Marcus (RRKM) theories of unimolecular reactions). Dynamics chain (hydrogenbromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen-bromine and hydrogen - chlorine reactions) and oscillatory reactions (Belousov- Zhabotinski reaction), homogeneous catalysis, kinetics of enzyme reactions. General features of fast reactions, study of fast reactions by flow methods, relaxation methods, Flash photolysis.

Unit-II

Chemical Thermodynamics and Phase Diagram: Phase rule, one and two component systems (solid-solid, solid-liquid, solid-vapor, liquid-liquid, liquid-vapor equilibrium), three component systems (Introduction and example). Ehrenfest classification of phase transitions. Phase diagram for semiconductors.

Unit-III

Statistical Thermodynamics: Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging, Canonical, grand canonical and microcanonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers) Partition functions-translational, rotational, vibrational and electronic partition functions, calculation of thermodynamic properties in terms of partition function.

Relevant Practicals/Demonstraions: Determination of Consolute Temperature for Phenol Water system, Determination of Partition Co-efficient of a solute in two different solvents, Determination of free energy and entropy from hydrolysis of ester.

Outcome: The students will get aquainted with the reaction dynamics and thermodynamics involved therein such that they can apply the same to various systems.

Text Book

Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 8th Edition, Oxford University Press (2006)

Recommended books & reference

1. Laidler, K. J. *Chemical Kinetics*, 3rd Edition, Pearson Education India (2003)
2. Houston, P. L. *Chemical Kinetics and Reaction Dynamics*, Dover Publications Inc (2006
3. S. Silbey, R. J., Alberty, R. A., Bawendi, M. G. *Physical Chemistry* 4th Edition, Wiley (2006)
5. McQuarrie, D. A. & Simon, J. D. *Physical Chemistry A Molecular Approach* Viva Books (2015)
6. McQuarie, D. A. *Statistical Mechanics* Viva Student Edition, Viva Books (2015)
7. Chandler, D. *Introduction to Modern Statistical Mechanics* Oxford University Press (1987)
8. Dill, K & Bromberg, S. *Molecular Driving Forces: Statistical Thermodynamics in Biology, Chemistry, Physics, and Nanoscience* 2nd Edition, Garland Science (2010)

Organic Photochemistry and Pericyclic Reactions CHM 621020

***Course Learning Objectives (CO)*: This course is intended to introduce students to photochemistry and pericyclic reactions.**

***Course Learning Outcomes (CLO)*: After the completion of the course, the students will have a comprehensive understanding of the development of scientific ideas about photochemistry and pericyclic reactions thus Creating, evaluating, analyzing, applying, understanding and remembering of photochemistry and pericyclic reactions.**

Course learning outcome:

After the completion of the course, the students will have a comprehensive understand of the development of scientific ideas in both thermal and photochemical concerted reactions.

CLO-1. To develop fundamentals of thermal and photochemical process with the formation of various excited state.

CLO-2. To learn various thermal and photochemical process through concerted mechanism.

CLO-3. To learn various photochemical reactions through concerted mechanism.

CLO-4. To analyse synthetic applications with hand on exercise in the laboratory.

Unit I: Aromaticity and Symmetry Controlled Reactions Symmetry properties of MOs. LCAO-MO theory of simple conjugated polyenes and cyclic polyenes. Aromaticity and antiaromaticity. Homo, hetero and nonbenzenoid aromatic systems. Aromaticity of annulenes. mesoionic compounds

Unit-II: Pericyclic Reactions, Molecular orbital symmetry, Frontier orbitals of ethylene 1,3 butadiene, 1,3,5, hexatriene and allyl system, classification of pericyclic reactions, Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions- conrotatory and disrotatory motion, 4n, 4n+2 and allyl systems. Cycloadditions – antarafacial and suprafacial addition ,4n and 4n+2 systems, 2+2 addition of ketenes, 1,3, dipolar cycloadditions. Sigmatropic rearrangements- suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3, and 5,5 sigmatropic rearrangements. Ene reaction.

Unit III: Organic Photochemistry & Free Radical Reactions Photochemical processes. Energy transfer, sensitization and quenching. Singlet and triplet states and their reactivity. Photoreactions of carbonyl compounds, enes, dienes, and arenes. Norrish reactions of acyclic ketones. Patterno-Buchi, Barton, photo-Fries and Di-pi-methane rearrangement reactions.

Unit IV: Photoreactions of Vitamin D. Photochemistry of vision and photosynthesis. Singlet oxygen generation and reactions. Applications of photoreactions and their applications for industrial synthesis.

Relevant Practicals/Demonstraions: Reaction of Anthracene with Maleic anhydride, Addition of oxygen

Recommended books and references

Organic reactions and orbital symmetry: T. L. Gilchrist and R. C. Storr, CUP Archive
Pericyclic reactions by S. M. Mukherjee
Pericyclic Reaction-A Text Book, S. Sankararamn, Wiley-VCH, Germany, 2005
Pericylic Reactions, Ian Fleming, Oxford Science Publications, New Delhi, 2011
Organic Photochemistry by J.M.Coxon and B. Halton, Cambridge Text in Chemistry
Orbital Symmetry: A Problem solving approach by R.E.Lehr and A.P. Marchand, Academic Press, New York, 1972.

Bioinorganic Chemistry CHM 621030

***Course Learning Objectives (CO)*: This course is intended to introduce students to the bioinorganic chemistry related to chemical kinetics, phase rule and statistical thermodynamics.**

***Course Learning Outcomes (CLO)*: After the completion of the course, the students will have a comprehensive understanding of the development of scientific ideas about bioinorganic chemistry thus Creating, evaluating, analyzing, applying, understanding and remembering of bioinorganic chemistry**

Unit-I:
Metalloenzymes, Iron enzymes – hemoglobin, myoglobin, Superoxide dismutase, catalase, peroxidase and cytochromes, Cyt-P450, hemocyanine, hemerythrine, non-heme iron enzymes, ferredoxin, Molybdenum oxatransferase. Ferritin, transferrin, and siderophores. Xanthine oxidase. Carbonic anhydrase, nitrate reductase. Vitamin B-12.
Unit II Nitrogen fixation and photosynthesis, biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidence, other nitrogenases model systems photosynthesis, active site of chlorophyll, photosystems.
Unit –III: Biochemical Processes in Living system, Phosphate hydrolysis, nucleotide transfer, DNA-polymerase, phosphate transfer, pyruvate kinase, glucose storage, phosphoglucomutase, phosphate storage in muscle, creatine kinase, NaK pump, ATPase. Metal ions / compounds as drugs, chelation therapy. Anticancer and antiarthritis drugs.

Recommended books and references
1. Principles of Bioinorganic Chemistry, S .J. Lippard and J. M. Berg., University Science Books, 1994.
2. Bioinorganic Chemistry, I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valenting, University Science Books.
3. Inorganic Biochemistry vols I and II ed. G. L.Eichhom, Elsevier
4. Progress in Inorganic Chemistry, Vols 18 and 38 ed J. J. Lippard, Wiley
5. Bioinorganic Chemistry, Asim K. Das, Books and Allied, 2nd Ed (2007).
6. Supramolecular Chemistry, J. W. Steed and J. L. Atwood, Willey, 2nd Ed (2009).
7. Bioorganic, Bioinorganic and Supramolecular Chemistry, P.S. Kalsi, J.P. Kalsi, New Age International, 2nd Ed (2012).
8. Bioinorganic Chemistry: Inorganic elements in the Chemistry of life., An Introduction and Guide—Wolfgang Kaim, Brigille Schwedrski John Wiley and sons, 1994

Analytical Chemistry CHM 621040

***Course Learning Objectives (CO)*: This course is intended to introduce students to analytical chemistry.**

***Course Learning Outcomes (CLO)*: After the completion of the course, the students will have a comprehensive understanding of the development of scientific ideas about analytical chemistry thus Creating, evaluating, analyzing, applying, understanding and remembering of analytical chemistry**

Unit-I: Errors, Statistics and Sampling

Accuracy, Precision, Types of errors – determinate and indeterminate errors, minimization of determinate errors, statistical validation- statistical treatment of finite data (mean, median, average deviation, standard deviation, coefficient of variation and variance), significant figures – computation rules, comparison of results – student's t-test, F-test, statistical Q test for rejection of a result, confidence limit, regression analysis – method of least squares, correlation coefficient, detection limits.

Unit-II: Chromatographic methods of analysis

Introduction, stationary phase, mobile phase, polarity of solvents, retention time, curve width, column adsorption equilibrium, gravity column chromatography, flash column chromatography, advantages and limitations of column chromatography. Gas Chromatography (GC): Introduction, instrumentation, types of columns (packed, open tubular etc.), types of detectors (TCD, ID, FID, ECD, element selective detectors), applications of GC for quantitative analysis. High performance liquid chromatography (HPLC): Introduction, Instrumentation, Types of liquid chromatography. Applications.

Unit-III: Spectroscopic Methods of Analysis UV-visible spectroscopy, Instrumentation, Calibration, Baseline Correction IR Spectroscopy: Instrumentation, sample handling, Fourier transform infrared spectroscopy Principle, instrumentation & its advantages. Raman Spectroscopy: Theory, Instrumentation, sample handling, Illumination diagnosis and structure analysis, polarization measurements, quantitative analysis. Principles of AAS, Instrumentation – flame AAS and furnace AAS, resonance line sources, sensitivity and detection limits in AAS, interferences –chemical and spectral, evaluation methods in AAS and application in qualitative and quantitative analysis. Atomic Emission Spectroscopy (AES): Principles of AES, Instrumentation, evaluation methods, Application in quantitative analysis.

Relevant Practicals/Demonstraions: Preparation of TLC, Separation using Column Chromatography, Varification of Beer-Lambert's Law

Recommended books and references:

1. Analytical Chemistry, G. D. Christian, 4 th Ed. John Wiley, New York (1986)
2. Instrumental methods of Analysis, H. H. Willard, L. L. Merritt, Jr J. A. Dean and F. A. Settle Jr 6th Ed CBS (1986).
3. Instrumental Methods of Analysis-G-Chatwal and S. Anand (Himalaya Publication;1988).
4. Introduction to Instrumentation Analysis by R.D. Braun Pharma Med Press.
5. Instrumental methods of chemical Analysis, B.K. Sharma, 16th edition Goel Publishing House.
6. Fundamentals of Analytical Chemistry, D. A. Skoog and D. M. West and F. J. Holler Holt-Saunders 6th Edition (1992).

7. Principles of Instrumental Analysis, D. A. Skoog, F. J. Holler and J.A. Niemann 5th Edition (1998)

Physical Chemistry Laboratory CHM 622060

Error Analysis and Statistical Data Analysis Errors, types of errors, minimization of errors, error distribution curves, precision, accuracy and combination; statistical treatment for error analysis, student 't' test, null hypothesis, rejection criteria, F & Q test; linear regression analysis, curve fitting.

Calibration of volumetric apparatus, burette, pipette and standard flask. Adsorption To study surface tension – concentration relationship for solutions (Gibbs equation)

Chemical Kinetics (i) Determination of the effect of (a) Change of temperature (b) Change of concentration of reactants and catalyst and (c) Ionic strength of the media on the velocity constant of hydrolysis of an ester / ionic reactions.
(ii) Determination of the velocity constant of hydrolysis of an ester / ionic reaction in micellar media.
(iii) Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide studying the kinetics as an iodine clock reaction.
(iv) Determination of the degree of dissociation of weak electrolyte and to study the deviation from ideal behaviour that occurs with a strong electrolyte. Electrochemistry A. Conductometry:
(v) Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide conductometrically.
(vi) Determination of solubility and solubility product of sparingly soluble (e.g., $PbSO_4$, $BaSO_4$) conductometrically.
(vii) Determination of the strength of strong and weak acids in a given mixture conductometrically.
(viii) Determination of the activity coefficient of zinc ions in the solution of 0.002 M zinc sulphate using Debye Huckel's limiting law. B. Potentiometry / pH metry: (i) Determination of strengths of halides in a mixture potentionmetrically.
(ix) Determination of the valency of Hg_2^{2+}ions potentiometerically.
(x) Determination of the strength of strong and weak acids in a given mixture using a potentiometer / pH meter.
(xi) Acid-base titration in a non-aqueous media using a pH meter.
(xii) Determination of the dissociation constant of acetic acid in acetone by titrating it with KOH in what medium.
(xiii) Determine the P^{Ka} of a dibasic acid by pH titration using a pH meter.

(xiv) Determination of rate constant for hydrolysis / inversion of sugar using a polarimeter.
(xv) Enzyme kinetics – inversion of sucrose.

Books Recommended

1. Practical Physical Chemistry, A. M. James and F.E. Prichard, Longman.
2. Findley's Practical Physical Chemistry, B. P. Levitt, Longman.
3. Experimental Physical Chemistry, R. C. Das and B. Behera, Tata McGraw Hill, 1983, New Delhi.
4. Vogel's Text book of Quantitative Analysis, revised, J.Bassett, R.C.Denney, G.H. Jeffery and J.Mendham, ELBS.
5. Fundamentals of Analytical Chemistry, D.A.Skoog, D.M.West and F.J.Hollar. 7th Edition, Harcourt College Publishers, 1996.

Seminar CHM 623060

SEMESTER-III	SEMESTER-IV

Sl no	Subject Code	Subject	Contact Hours per week (L+T+P)	Credits
1		Organometallic Chemistry	3+1	4
2		Group Theory, Molecular Spectroscopy and Surface Chemistry	3+1	4
3		Main Group Chemistry, Actinides, Lanthanides and Nuclear Chemistry	3+!	4
4		MOOCs I (Organic reaction mechanism)	4	4
5		Analytical Chemistry Practical	2	2
6		Minor Project	4	4
TOTAL CREDITS				**22**

Sl no	Subject Code	Subject	Contact Hours per week (L+T+P)	Credits
1		Major Project		20
2		MOOCs II		4
3				
TOTAL CREDITS				**24**

Organometallic Chemistry

***Course Learning Objectives (CO)*: This course is intended to introduce students to organometallic chemistry.**

***Course Learning Outcomes (CLO)*: After the completion of the course, the students will have a comprehensive understanding of the development of scientific ideas about organometallic chemistry thus Creating, evaluating, analyzing, applying, understanding and remembering of organometallic chemistry**

Self-Study:

Definition, Classes of ligands, haptacity, 18-electron rule and its applications. Metal-alkene, Metal-alkyne complexes, metal-dinitrogen compounds: Zeises salt (preparation, structure and bonding), Sandwich molecules, Ferrocene (preparation, structure and reactions).

Unit-I

Metal Carbonyls and Nitrosyls: Structure, nature of bonding, interpretation using IR spectroscopy, syntheses and reactivity.
Metal-phosphines: Structure, nature of bonding, steric and electronic parameter, basicity of phosphines.
Metal carbenes: Classification (Fischer carbenes and Schrock carbenes), Structure, nature of bonding, syntheses, reactivity and applications.
Tebbe's reagent: preparation and its applications.
N-heterocyclic carbenes: Preparation, bonding nature with transition metals and reactivity. Metal-cyanide, Metal-isocyanides

Unit-II

Study of Organometallic Compounds: Organo-magnesium, Organo-aluminium, Organo-zinc and Organo-lithium, Organo cupper reagents, Corey-House synthesis, Gilman reagents and its applications.

Metathesis: Definition, synthetic tool, synthesis of metathesis catalysts (Grubbs' and Schrock), mechanism of ring opening metathesis (ROM), cross metathesis (CM), ring closing metathesis (RCM), ring opening metathesis polymerization (ROMP) and enyne metathesis (EM). Few applications

Unit-III

Basic organometallic reaction mechanism: Oxidative addition, Reductive elimination, Migratory insertion, Alkene insertion, β-hydride elimination, Transmetallation. **Pd, Cu, Ni cross coupling reactions:** The Heck reaction, Suzuki-Miyaura, Sonogashira, Stille, Kumada, Negishi, Hiyama coupling, Buchwald-Hartwig C-N cross coupling, Fukuyama coupling, Chan Lam coupling, Ullmann Reaction, Cadiot-Chodkiewicz Coupling, Glaser Coupling, Eglinton Reaction. Olefin polymerization, Oxo, Wacker processes, Monsanto acetic acid, Ziegler-Natta, ZSM, Catalytic cycle of Wilkinson's catalyst; Iridium/Ruthenium based catalysts for asymmetric hydrogenation.

Recommended books

1. "Organometallic Chemistry of the Transition Metals", R. H. Crabtree, Wiley, New York, 1988.
2. "Organometallics: A Concise Introduction", C. Elschenbroich and A. Salzer, 3rd Edn.1999.
3. "Basic Organometallic Chemistry" B D Gupta, A J Elias, 2nd Edn. 2013, Universities Press

Group Theory, Molecular Spectroscopy and Surface Chemistry

***Course Learning Objectives (CO)*: This course is intended to introduce students to group theory, molecular spectroscopy and surface chemistry.**

***Course Learning Outcomes (CLO)*: After the completion of the course, the students will have a comprehensive understanding of the development of scientific ideas about group**

theory, molecular spectroscopy and surface chemistry thus Creating, evaluating, analyzing, applying, understanding and remembering of group theory, molecular spectroscopy and surface chemistry

Unit-I: Group theory:

Symmetry elements and Symmetry operation, Groups and Subgroups, Point group. Schonflies notation, matrix representations of groups, irreducible representations and character tables. The Great Orthogonality theorem and its importance. Derivation of character table. Application of group theory in Quantum Mechanics, Chemical Bonding, Metal Complexes, Spectroscopy

Unit-II: Molecular Spectroscopy:

The rigid diatomic rotor, energy eigenvalues and eigenstates, selection rules, intensity of rotational transitions, the role of rotational level degeneracy, the role of nuclear spin in determining allowed rotational energy levels. Classification of polyatomic rotors and the non-rigid rotor. Vibrational spectroscopy, harmonic and anharmonic oscillators, Morse potential, mechanical and electrical anharmonicity, selection rules. The determination of anharmoncity constant and equilibrium vibrational frequency from fundamental and overtones. Normal modes of vibration, internal and symmetry coordinates. Basics of Raman spectroscopy, Electron Spin Resonance Spectroscopy, Mossbauer Spectroscopy.

Unit-III: Surface Chemistry:

Adsorption, Surface tension, capillary action, pressure difference across curved surface, vapour pressure of droplets. Gibbs adsorption isotherm, estimation of surface area (BET equation), surface films on liquids (Electrokinetic phenomenon), catalytic activity at surfaces. Surface active agents, classification of surface-active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants counter ion binding to micelles, thermodynamics of micellization, phase separation and mass action models, solubilization, micro emulsion, reverse micelles.

Self-Study:

1. Recognizing the significance and utilizing group theory in chemical systems
2. Discern the connection between classical and statistical thermodynamics.
3. Probe into the physical properties of molecules.

Recommended Textbooks / references:

1. Cotton, F. A. Chemical Applications of Group Theory 3rd Edition, Wiley (2008).
2. Carter, R. L. Molecular Symmetry and Group Theory Wiley Student Edition, Wiley (2009).
3. Bishop, D. M. Group Theory and Chemistry Dover Publications Inc (1993)

4. McQuarie, D. A. Statistical Mechanics Viva Student Edition, Viva Books (2015)5. Chandler, D. Introduction to Modern Statistical Mechanics Oxford University Press (1987)
6. Dill, K & Bromberg, S. Molecular Driving Forces: Statistical Thermodynamics in Biology, Chemistry, Physics, and Nanoscience 2nd Edition, Garland Science (2010)
7. Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry 8th Edition, Oxford University Press (2006).
8. Silbey, R. J., Alberty, R. A., Bawendi, M. G. Physical Chemistry 4th Edition, Wiley (2006

Main Group Chemistry, Actinides, Lanthanides and Nuclear Chemistry

***Course Learning Objectives (CO)*: This course is intended to introduce students to main group chemistry.**

***Course Learning Outcomes (CLO)*: After the completion of the course, the students will have a comprehensive understanding of the development of scientific ideas about main group chemistry thus Creating, evaluating, analyzing, applying, understanding and remembering of main group chemistry**

Unit-I: Stereochemistry and Bonding in main group compounds VSEPR, Walsh diagram (tri molecules), dz-Pp bonds, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules. General characteristics, Allotropes, Structure and Reactions of simple and industrially important compounds: Boranes, Carboranes, Silicones, Silicates, Boron nitride, Borazines and Phosphazenes.

Unit-II: General characteristics, Structure and Reactions of simple and industrially important compounds: Hydrides, Halides, Oxides and Oxoacids of pnictogens (N, P), chalcogens (S, Se & Te) and halogens, Xenon compounds, Pseudo halogens and Interhalogen compounds.

Unit-III: Lanthanides, actinides, extraction, separation, purification, application, contractions and its significance, post actinide elements, radioactive elements, half-life, disintegration, radiocarbon dating, tracer techniques, and use in medicinal, agricultural and structural interpretations, nuclear reactions as source of energy.

Relevant Practicals/Demonstraions:

1. Separation of few lanthanides by fractional crystallization, and elution chromatography, determination of Rf.
2. Estimation of halides and pseudo-halides using argentometric titration using indicators.
3. Estimation of nitrate, phosphate, borate, and sulphate in unknown samples.

Recommended books & references:

1. Chemical Application of Group Theory: F. A. Cotton, John Wiley.
2. Symmetry in Chemistry: Orchin and Jaffe.
3. Group theory: K. V. Raman, Tata McGraw Hill.
4. Advanced Inorganic Chemistry: F. A. Cotton and G. Wilkinson, John Wiley.
5. Inorganic Chemistry: J.E. Huheey, E. A. Keiter, R. L. Keiter, Pearson Education.
6. Chemistry of the Elements: N. N. B. Greenwood and A. Earnshow, Pergamon
7. Comprehensive Coordination Chemistry eds,- G. Wilkinson, R. D. Gillars and J A. McCleverty, Pergamon.
8. Fundamental concepts of Inorganic Chemistry – A. K. Das (Vol 2), CBS.
9. General and Inorganic Chemistry- Part 2, R. Sarkar, Central pubication
10. Inorganic Chemistry – Wulfsberg, Viva.

MOOCs I (Organic reaction mechanism)

UNIT I
Broad classification of reactions and basics of arrow pushing, Reaction co-ordinate diagrams Reaction Kinetics: rate laws and methods of determining concentration. Introduction to linear free energy relationships, Linear Free Energy Relationships.

UNIT II
Kinetic and equilibrium isotope Effects, Miscellaneous methods to determine mechanisms: isotope labelling, trapping of intermediates, checking for common intermediate, competition and cross-over experiments.

UNIT III
Catalysis: classification and introduction to Bronstead acid catalysis, Types of Catalysis: Acid, Binding, Electrophilic, Nucelophilic, Covalent, Proximity and Phase-transfer

Analytical Chemistry Practical

1. Analysis of Bronze with respect to Copper and Tin
2. Analysis of Dolomite ore for Ca, Mg and Silicate material
3. Analysis of Cement with respect to SiO_2, Calcium, Iron, Magnesium and Aluminium
4. Spectrophotometric determination of lead in leaves using dithizone-chelating agent
5. Determination of alcohol from given sample spectrophotometrically
6. Determination of Nitrogen from Fertilizer sample
7. Determination of Phosphate from fertilizer sample by volumetric method.
8. Removal of dyes on activated charcoal by column chromatography
9. Determination of COD from waste water
10. Analysis of water with respect to sulphate & Chloride
11. Determination of organic carbon in soil

Minor Project

Semester IV

MOOCs II

Major Project

In the final semester (IV^{th} semester), students have to carry out project work at CUJ as per the recommendation of faculty committee of the Department/centre under the supervision of a scientist/Faulty member. Joint collaboration with other Departments/centres/schools is encouraged in order to enhance the quality of work and interdisciplinary characteristics in the work. The Area of the work is to be decided by the Adviser(s). On completion of the Project work, students have to submit their work in the form of a dissertation followed by oral presentation in the presence of Faculty members and an external expert member.