M.Sc. (Chemistry)

SYLLABUS FOR TWO-YEAR FULL-TIME PROGRAMME

(Four Semester Course)

Department of Chemistry

MADHABDEV UNIVERSITY

Narayanpur-784 164, Assam, India

SEMESTER I

Title of the Course: Inorganic Chemistry-I
Course Code: PCHC-101
Total Credits: 4
Distribution of Marks: 100 (End Sem 60 + Internal Assessment 40)

Course Objective: In this introductory course on inorganic chemistry, students will be able to understand the importance inorganic cages and clusters, gain insight into acid base concept in Inorganic Chemistry and will provide a broad foundation in inorganic biochemistry.

Learning Outcome: Students will be able to explain/describe/rationalize inorganic cages and clusters, will develop concepts on acid base chemistry from the inorganic chemistry perspective and will gather knowledge about role of different metals and nonmetals in biological system.

UNIT I: **Inorganic Cages and Clusters**

Structure and bonding in polyhedral boranes, carboranes, metalloboranes and metallocarboranes, styx notation; Wade's rule; electron count in polyhedral boranes; synthesis of polyhedral boranes. Synthesis, structure and bonding in borazines, phosphazenes, sulphur-nitrogen compounds, siloxanes, iso- and hetero-poly anions. Structure and chemistry of silicates, aluminosilicates, zeolites and clays.

Lecture 15, Marks 20

UNIT II: Acid Base and Redox Chemistry

Acid-Base concepts, Measure of Acid-Base Strengths, Acid-Base in water. Non-aqueous solvent, aprotic solvent and superacids. Hard and Soft Acids and Bases, application of HSAB principle.

Half cell reaction, reduction potential, application of reduction potential data, electrochemical series; brief idea of corrosion and its prevention; Nernst equation. Latimer and Frost diagram (V, Mn Fe, Cu etc.), disproportionation reaction; cyclic voltametry.

Lecture 20, Marks 20

UNIT III: Bioinorganic Chemistry

Fundamentals of inorganic biochemistry, essential, non-essential and role of 3d block elements and non-metals in bio-systems.

Natural and synthetic oxygen carriers, Porphyrins, model compounds for oxygen binding and carriers: Hemoglobin, myoglobin, hemerythrin, hemocyanin, Electron transfer protein: Cytochromes, Iron-Sulphur, Nitrogen fixation. Metalloenzymes, corrinoids (vitamin B12 and co-enzyme), carboxy-peptidases, chlorophyll and photosynthesis, Na-K or ATPase or sodium pump, crown ethers, futuristic aspects of organo-transition metal complexes in bioinorganic chemistry.

Lecture 25, Marks 20

Recommended Books

1. Housecroft, C. E; Sharpe, A. G., Inorganic Chemistry, 5th Ed., Pearson Education, Essex (2018).
2. Atkins, P.; Overton, T.; Rouke, J.; Weller, M.; Armstrong, F.; Hagerman, M., Shriver Atkins's Inorganic Chemistry, 6th Ed., Oxford University Press, New Delhi (2015).
3. Miessler, G.; Tarr, D. A., Inorganic Chemistry, 3rd Ed., Pearson Education India, New Delhi (2008).
4. Huheey, J. E.; Keiter, E. A.; Keiter, R. L.; Medhi, O. K., Inorganic Chemistry: Principles of Structures and Reactivity, 4th Ed., Pearson Education India, New Delhi (2006).
5. Kaim, W.; Schwederski, B.; Klein, A., Bioinorganic Chemistry-Inorganic Elements in the Chemistry of Life: An Introduction and Guide, 2nd Ed., John Wiley & Sons, West Sussex (2013).
6. Bertini, I.; Gray, H. B.; Lippard, S. J.; Valentine, J. S., Bioinorganic Chemistry, Viva Books, New Delhi (2007).

Further Reading

1. Cotton, F. A.; Bochmann, M.; Murillo, C. A.; Wilkinson, G., Advanced Inorganic Chemistry, 6th Ed., Wiley India, New Delhi (2007).
2. Rehder, D., Bioinorganic Chemistry, Oxford University Press, London (2014)
3. Roat-Malone, R. M., Bioinorganic Chemistry: A Short Course, 2nd Ed., Wiley Blackwell, New York (2007).
4. Reddy, K. H., Bioinorganic Chemistry, New Age International Publishing, New Delhi (2009).

SEMESTER I

Title of the Course: Organic Chemistry-I
Course Code: PCHC-102
Total Credits: 4
Distribution of Marks: 100 (End Sem 60 + Internal Assessment 40)

Course objective: In this course on organic chemistry, students will be introduced to conceptual organic chemistry, stereochemistry of organic molecules, reaction mechanisms and the intermediates.

Learning outcome: Students will be able to appreciate/demonstrate/explain the unique features of organic reactions mechanism, reaction intermediates and stereochemistry, and solve related problems.

UNIT I:

Basic Stereochemistry

Stereoisomerism in organic compounds: brief introduction of geometrical and optical isomerism. Interconversions of projection formulae, Conformational analysis of simple cyclic and acyclic systems, butane- gauche and 1,3-diaxial interactions and their influences in stability of molecules. Optical purity, optical activity in absence of chiral centre: chiral axis, chiral plane and helical chirality. Asymmetry and dissymmetry: Concept of stereogenic, chirotopic and achirotopic centres; prochirality (Re- & Si face), prosterioisomerism; homotopic and heterotopic faces; diastereomerism in acyclic and cyclic systems.

Lecture 12, Marks 12

UNIT II: Structure, bonding and reactivity of organic compounds :

Aromaticity, antiaromacity and homoaromaticity, metallocenes, tropolones and azulenes. Supramolecularchenmistry: Bonds weaker than covalent bond – charge transfer complexes, inclusion complexes and crown ethers. Cryptand, rotaxanes, Fullerenes, Graphenes. Phase transfer catalyst. Hammet equation, Taft equation. Influence of reaction medium on rates.

Lecture 12, Marks 12

UNIT III: Organic reaction mechanism

Transition state vs. Reaction intermediate, Energy profile of multistep reaction, Significance of rate limiting step in multistep reactions, Catalysed and uncatalysed reactions, Kinetic vs. Thermodynamic control, Kinetic and non-kinetic methods of studying organic reaction mechanism; Isotope labeling studies and kinetic isotope effects, Cross-over experiment.

Reactivity - selectivity principle :Chemoselectivity, regioselectivity, stereoselectivity and stereospecificity in substitution, elimination and addition reactions. Neighbouring group effects. Organic reactive intermediates: Generation, stability and reactivity of carbocations, carbanions, free radicals, carbenes, benzynes and nitrenes.

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Lecture 12, Marks 12

UNIT IV: Ionic Reaction Intermediates

Carbocation: Generation, structure and reactivity, classical and non-classical carbocations, neighbouring group participation and rearrangements in acyclic, monocyclic and bicyclic systems. Carbanions: Generation, structure and reactivity. Organolithium, organomagnesium, organozinc, organocopper reagents. Enolates: Themodynamic versus kinetic enolates, enolate equivalent and enamines: Application in carbon-carbon bond formation and other reactions. Cram's rule, Felkin-Anh model, Zimmerman-Traxler model. Ylides: Chemistry of phosphorous and sulfur ylides – Wittig reaction: stabilized and non-stabilised ylides, related reactions, Petersen olefination.

Lecture 12, Marks 12

UNIT IV: Non-ionic Reaction Intermediates

Free radicals: Generation, structure, stability and reactions, radical initiator, cage effects, radical cations and radical anions, application of tributyltinhydride/AIBN, Hoffmann Loeffler-Freytag reaction and Barton reaction. Carbenes: Formation, structure and stability, singlet and triplet states, Reimer-Tiemann and other reactions involving carbene intermediate. Nitrenes: Generation & structure, reactions of nitrenes and related electron deficient nitrogen intermediates. Arynes: Generation, structure and stability, rearrangement reactions, SNAr mechanism.

Lecture 12, Marks 12

Recommended Books

1. Smith, M. B.; March, J., March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 7th Ed., Wiley India, New Delhi (2015).
2. Greeves, N.; Clayden, J.; Warren, S., Organic Chemistry, 2nd Ed., Oxford University Press, New Delhi (2012).

3. Nasipuri, D. Stereochemistry of Organic Compounds: Principles and Applications, 3rd Ed., New Age International Publishers, New Delhi (2018).

Further Reading

1. Smith, M. B., Organic Synthesis, 4th Ed., Academic Press, Cambridge, Massachusetts (2016).
2. Sengupta, S., Basic Stereochemistry of Organic Molecules, 2nd Ed., Oxford University Press, New Delhi (2018).
3. Kalsi, P. S., Stereochemistry: Conformation and Mechanism, 10th Ed., New Age International Publishers, New Delhi (2019).

SEMESTER I

Title of the Course: Physical Chemistry-I
Course Code: PCHC-103
Total Credits: 4
Distribution of Marks: 100 (End Sem 60 + Internal Assessment 40)

Course Objective: In this course on physical chemistry, students will introduced to the fundamentals of chemical thermodynamics, quantum chemistry and molecular spectroscopy.

Learning Outcome: Students will understand the fundamentals and develop skills to solve problems related chemical thermodynamics, and spectroscopy.

UNIT I: Chemical thermodynamics

Brief resume of law of thermodynamics; Gibbs and Helmholtz free energy functions and their significance. Thermodynamic criteria for the processes in terms of entropy change, internal energy change, enthalpy and free energy (Gibbs and Helmholtz) change. Gibbs – Helmholtz equation and its utility in thermodynamics of reaction. Fugacity and activity and their variation with temperature and pressure. Graphical method for the determination of fugacity; fugacity of van der Waals gases. Partial molar quantities and its physical significance; Partial molar free energy (chemical potential) and its variation with temperature and pressure; Gibbs-Duhem equation. Gibbs free energy and entropy of mixing of ideal gases; partial molar volumes; method of determination of partial molar volumes. Thermodynamic description of phase transitions and Clapeyron-Claussius equation.

Lecture 15, Marks 15

UNIT II: Quantum Chemistry-I

Review of the basic principles of Quantum Mechanics: Postulates, Linear and Hermitian operators, commutation relation, related important theorems.

Model Systems: Free particle and particle in a box (One and three dimensional), degeneracy. Simple Harmonic Oscillator-Schrodinger equation and its solution, Hermite polynomials, two-particle rigid rotor- rotational energy levels of diatomic molecules, particle in a ring, quantum mechanical tunnelling.

Lecture 15, Marks 15

UNIT III: Spectroscopy

Electromagnetic spectrum, Interaction of emr with matter, Natural line width and Broadening- Intensity of spectral transitions. Selection rules. Rotational (microwave) spectroscopy: Classification of molecules according to their moments of inertia, rotational energy levels of HCl, Selection rule for Microwave spectra, intensity, effect of substitution in Microwave spectra. Stark effect, spectra of symmetric top and asymmetric top type molecules. Fundamental vibrational frequencies, Selection rules and vibrational energy for harmonic and

anharmonic oscillators, vibration rotational spectra of diatomic molecules, Fundamental, overtone and combination bands, P, Q and R branches, hot bands, group frequencies, normal modes of vibrations, symmetry of vibrations. Quantum theory of Raman effect, Selection rules, mutual exclusion principle, vibration-rotation Raman spectra. Intensity of Raman lines. Electronic spectroscopy: Electronic transitions and selection rules, Frank Condon principle and electronic spectra of polyatomic molecules, Fluorescence and phosphorescence, solvent effects, absorption and intensity shifts, Calculation of absorption maxima by Woodward-Fieser

Rules.

Lecture 30, Marks 30

Recommended Books:

1. Physical Chemistry by P.W. Atkins
2. Quantum Chemistry, by Ira N. Levine, Pentice Hall
3. Fundamentals of Molecular Spectroscopy by C.N. Banwell and E.M. McCash, Tata McGraw Hill.

Further Reading

1. Physical Chemistry by I. N. Levine
2. Thermodynamics for Chemist by S. Glasstone
3. Introduction to Quantum Chemistry by A.K. Chandra, Tata McGraw Hill.
4. Molecular Quantum Mechanics by P.W. Atkins & R.S. Friedman, Oxford University Press.
5. QuantumChemistry, byD.A. McQuarrie, VivaBooksPvt.Ltd.:NewDelhi
6. Introduction to Molecular Spectroscopy by G.M. Barrow, McGraw Hill.

SEMESTER I

Title of the Course: Inorganic Chemistry Laboratory
Course Code: PCHC-104
Total Credits: 6
Distribution of Marks: 150 (End Sem 90 + Internal Assessment 60)

Course Objective: This core laboratory course in inorganic chemistry would expose students to experimental skills of qualitative and quantitative analysis and synthesis of coordination compounds with selected examples. Spectroscopic techniques like UV-visible, infrared, fluorescence etc. and other characterization techniques such as magnetic susceptibility and electrical conductivity measurements will be introduced.

Learning Outcome: From this course, the students will be able to perfect experimental skills encompassing synthesis, characterization of different inorganic compounds. Students will learn to use instruments like UV-visible and FT-Infrared, fluorescence spectrophotometer through hand-on training.

A. Preparation and characterization (viz. conductivity measurement, IR, UV-Vis) of the following complexes:

1. Potassium chromioxalate, $K_3[Cr(C_2O_4)_3]$
2. Reinecke's salt
3. Tris-(thiourea) copper(I) sulphate, $[Cu(tu)_3]2SO_4.2H_2O$
4. Potassium chromithiocyanate
5. Chloropentamine Cobalt (III) chloride $[Co(NH_3)_5Cl]Cl_2$
6. NitropentamineCobalt(III) chloride $[Co(NO_2)(NH_3)_5]Cl_2$

Marks 25

Viva 5

B. 1. Synthesis and characterization (melting point, conductivity, IR, UV-vis etc.) of Ni-DMG complex and estimate the percentage of nickel in the synthesized compound.

2. Synthesis and characterization of Schiff-base ligands and their metal complexes.

3. Synthesis and characterization of metal and metal oxide nanoparticles by surfactant assisted methods.

Marks 25

Viva 5

C. 1. Synthesis and characterization (melting point, conductivity, IR, UV-vis etc.) of trans-triglycinatoCu(II) monohydrate and estimate the percentage of 'Cu' in the synthesized compound.

2. Synthesis and characterization of Schiff-base ligands and their metal complexes.

3. Synthesis and characterization of magnetic nanoparticles by surfactant assisted methods.

Marks 25

Viva 5

Recommended Books:

1. Mendham, J.; Denney, R. C.; Barnes, J. D.; Thomas, M.; Sivasankar, B., Vogel's Textbook of Quantitative Chemical Analysis, 6th Ed., Pearson Education, New Delhi (2009).

2. Raj, G., Advanced Practical Inorganic Chemistry, Krishna Prakashan, Meerut (2013).

SEMESTER II

Title of the Course: Inorganic Chemistry-II
Course Code: PCHC-201
Total Credits: 4
Distribution of Marks: 100 (End Sem 60 + Internal Assessment 40)

Course Objective: In this course on inorganic chemistry, students will learn the chemistry of transition metal complexes, and f-block elements. They will learn the importance of inorganic reaction mechanism.

Learning Outcome: Students will be able to explain/describe/rationalize about the chemistry of transition metal complexes, and f-block elements and will gather knowledge about importance of inorganic reaction mechanism.

UNIT I: **Chemistry of Transition metal complexes**

Part A: ***Bonding in Transition Metals***

Crystal field theory of bonding in octahedral, JT-distorted octahedral, square planar, square pyramidal, trigonal bipyramidal, and tetrahedral complexes; CFSE for d^1 to d^{10} systems, pairing energy, low-spin and high-spin complexes. Ligand Field Theory (LFT) and molecular orbital (MO) theory of selected octahedral and tetrahedral complexes; thermodynamic aspects of LFSE.

Part B: ***Electronic spectra of Transition Metal-Complexes***

Electronic states and terms for transition metals. Selection rules, Orgel diagram and Tanabe-Sugano diagrams. Application in transition metal electronic spectroscopy. Electronic spectra and structure, d-d and charge transfer transitions.

Lecture 20, Marks 20

UNIT II: Magnetochemistry

Types of magnetic bodies (e.g, Diamagnetic, Paramagnetic, ferromagnetic and antiferromagnetic), antiferromagnetic coupling, Magnetic properties based on crystal field theory: spin only magnetic moments, spin-state equilibrium in octahedral stereochemistry: cross-over region, quenching of orbital magnetic moment by CF, orbital contribution, effect of temperature on magnetic behaviour, magnetic properties of octahedral, tetrahedral, tetragonally distorted octahedral and sequence planer complexes.

Lecture 10, Marks 10

UNIT III: Inorganic reaction mechanism

Lability and inertness, stability constant- formation constant of complexes, chelate effect, Thermodynamic and Kinetic stability; inert and labile complexes; Factor affecting stability, Correlation of stability constant with thermodynamic factors –G, H and S. Determination of stability constant –Jobs and Bjerrum's methods. Mechanism of ligand replacement reactions: Substitution reactions in octahedral [Cr(III), Co(III)] and square planar [Rh(I), Pt(II) and Pd(II)] complexes, Rate of water replacement reaction; Solvolysis and hydrolysis reaction; acid hydrolysis and base hydrolysis reaction; Factors affecting the rate of substitution reaction, trans effect and its importance, theories of trans effect, idea concerning electron transfer reactions, inner and outer sphere reactions..

Lecture 20, Marks 20

UNIT IV: Chemistry of Lanthanides and Actinides

Electronic configuration, lanthanide contraction, separation of lanthanides, Magnetic and spectral properties of lanthanides and actinides, lanthanide shift reagents. Stability of lanthanide and actinide complexes.

Lecture 10, Marks 10

Recommended Books

1. Housecroft, C. E; Sharpe, A. G., Inorganic Chemistry, 5th Ed., Pearson Education, Essex (2018).
2. Atkins, P.; Overton, T.; Rouke, J.; Weller, M.; Armstrong, F.; Hagerman, M., Shriver Atkins's Inorganic Chemistry, 6th Ed., Oxford University Press, New Delhi (2015).
3. Miessler, G.; Tarr, D. A., Inorganic Chemistry, 3rd Ed., Pearson Education India, New Delhi (2008).
4. Huheey, J. E.; Keiter, E. A.; Keiter, R. L.; Medhi, O. K., Inorganic Chemistry: Principles of Structures and Reactivity, 4th Ed., Pearson Education India, New Delhi (2006).

Further Reading

1. Cotton, F. A.; Bochmann, M.; Murillo, C. A.; Wilkinson, G., Advanced Inorganic Chemistry, 6th Ed., Wiley India, New Delhi (2007).
2. Figgis, B. N.; Hitchman, M. A., Introduction to Ligand Field Theory and Its Applications, Wiley India, New Delhi (2010).

SEMESTER II

Title of the Course: Organic Chemistry-II
Course Code: PCHC-202
Total Credits: 4
Distribution of Marks: 100 (End Sem 60 + Internal Assessment 40)

Course Objective: In this course will introduce different biomolecules and their bio-functioning mechanisms and also provide knowledge on applications of NMR and Mass spectrometry in combination with other spectroscopic techniques for analysis of molecular compounds.

Learning Outcome: Students will achieve insight on isolation, characterization and synthesis of various natural compounds of biological importance and able to analyse molecular compounds using different spectroscopic techniques.

UNIT I: **Enzymes and Co-enzymes:**

Classification of enzymes; Chemical nature of enzyme, Specificity of enzyme, Mechanism of enzyme action, Factors effecting enzyme action, Mechanism of action of chymotrypsin. Co-enzymes, co-factors, prosthetic groups: Mechanism of action of NAD+ , NADP+ , FMN, FAD. Functions of ATP. Nucleic acids: Review on chemical constitution and biological role of nucleic acids. Double heical structure of DNA. Chemical basis of heredity, Genetic code, Replication of DNA.Transcription and translation. Biosynthesis of proteins, Chemical synthesis of DNA, PCR.

Lecture 12, Marks 12

UNIT II: Alkaloids:

Occurance, classification, general methods of isolation, test for detection. Structure elucidation by physical and chemical methods and synthesis (including retrosynthetic approach) of :Piperine, Papaverine, Atropine and Morphine. Terpenoids: Occurance and classification, isoprene rule, general methods of isolation. Biogenetic pathway of mono- and sesquiterpenes. Structure determination by physical and chemical methods and synthesis of the following: Acyclic monoterpenoid – Linalool. Monocyclic monoterpenoid -Terpeneol, Menthol, Bicyclic monoterpenoid: pinene, Camphor, Borneol.

Lecture 12, Marks 12

UNIT III: Carbohydrates:

Structure, reaction and conformation of disaccharides – sucrose, maltose and lactose. Polysaccharides – starch and cellulose.

Peptides and Proteins : Structure determination and synthesis of small peptides (di-, tri- and tetra-). Solid phase synthesis of peptides.Classification of proteins.Primary, secondary and tertiary structure of proteins.

Lecture 12, Marks 12

UNIT IV NMR spectroscopy:

Chemical shift, factors affecting chemical shift, spin- spin interaction, Coupling constant and Factors affecting, relaxation processes, NOE, Nuclear magnetic double resonance, shift resonance, spin tickling; Proton and 13C NMR spectroscopy of simple organic molecules, living systems – MRI, : Two dimensional NMR, NOESY, DEPT, INEPT terminology, Instrumentation, FT NMR. IR: Application of IR in organic spectroscopy

Lecture 12, Marks 12

UNIT V: Mass spectrometry:

Ion fragmentation mechanism, Base peak and molecular ion peak, metastable peak, instrumentation and techniques, ionization methods, isotopic distribution, Application in determining the structure of organic and inorganic compounds Spectroscopic methods in analysis of molecular composition/Structure: Use of IR, electronic, 1H, 13C &31P NMR, Mass spectrometry.

Lecture 12, Marks 12

Recommended Books

1. Berg, J. M.; Tymoczko, J. L.; Gatto Jr., G. J.; Stryer, L., Biochemistry, 9th Ed., W. H. Freeman, New York (2019).

2. Voet, D.; Voet, J. G., Pratt, C. W., Biochemistry, 4th Ed., John Wiley and Sons, New Jersey (2012).

3. Silverstein, R. M.; Webster, F. X.; Kiemle, D. J.; Bryce, D. L., Spectrometric Identification of Organic Compounds, 8th Ed., Wiley India, New Delhi (2015).

4. Kemp, W., Organic Spectroscopy, 3rd Ed., Macmillan Publishers India, New Delhi (2011).

Further Reading

1. Campbell, M. K.; Farrell, S. O., Biochemistry, 8th Ed., Brooks/Cole, Belmont (2015).

2. Nelson, D. L.; Cox, M. M., Lehninger Principles of Biochemistry, 7th Ed., W. H. Freeman, New York (2017).
3. Gunther, H., NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry, 2nd Ed., Wiley India, New Delhi (2010).
4. Dyer, J. R., Applications of Spectroscopy of Organic Compounds, PHI Learning, New Delhi (2004).

SEMESTER II

Title of the Course: Physical Chemistry-II
Course Code: PCHC-203
Total Credits: 4
Distribution of Marks: 100 (End Sem 60 + Internal Assessment 40)

Course Objective: In this course will impart knowledge on the Schrodinger equation of Hydrogen atom and approximations applicable to more complex systems, thermodynamics of adsorption, kinetics of heterogeneous catalysis, electrical aspects of surface chemistry, basics of reverse micelle and microemulsions and concept of statistical thermodynamics.

Learning Outcome: Students will be able to solve the Schrodinger equation for Hydrogen atom and will be able to apply appropriate approximations to systems with more than one electron. Students will also understand the concepts of surface chemistry and statistical thermodynamics.

UNIT I: Quantum Chemistry-II

Hydrogen atom- Schrodinger equation, separation of relative coordinates, radial solution, probability and radial distribution function, angular solution, representation of orbitals, degeneracy, orbital and spin angular momentum. Approximate methods: Variation theorem, Linear variation functions. Time independent Perturbation theory for non-degenerate systems (up to second order in energy); application to the helium atom.Hellmann-Feynmann theorem. Antisymmetry Principle, Slater determinant, Term symbol, spectroscopic states. Born-Oppenheimer approximation, LCAO-MO and VB treatment of the Hydrogen molecule and Hydrogen molecule ion, Comparison of Molecular Orbital and Valence Bond Methods. Huckelmolecular orbital theory: Postulates, application to ethylene, butadiene, and benzene. Introduction to extended Huckel theory.

Lecture 24, Marks 30

UNIT II: Surface Chemistry

Thermodynamics of adsorption processes, Adsorption isotherms: Langmuir and BET. Determination of surface area of an adsorbent. Capillary condensation – adsorption in micropores, hysteresis loop. Kinetics and Mechanism of heterogeneous catalysis–Langmuir-Hinshelwood model, Eley-Riedel model, unimolecular and bimolecular surface reaction, Chemisorption: Chemisorption on metals, semi-conducting oxides and insulator oxides. Electrical aspects of surface chemistry, Electro kinetic phenomena, the structure of electrical

double layer, Zeta potential and colloidal stability, Measurement of zeta potential. Surfactants – definition and classification, micelle formation and determination of critical micelle concentration. Reverse micelle and its application, solubilization, microemulsion.

Lecture 12, Marks 15

UNIT III: Statistical Thermodynamics

Probability and most probable distribution, distinguishable and indistinguishable particles, Concept of ensembles, partition functions and distributions, microcanonical, canonical and grand canonical ensembles, Boltzmann distribution, Elementary idea of Fermi-Dirac and Bose-Einstein distributions. Ideal gases: Canonical partition function in terms of molecular partition function of non-interacting particles, Translational, rotational and vibrational partition functions. Absolute values of thermodynamic quantities (U,H,S,A) for ideal monoatomic and diatomic gases, heat capacity (Cv, Cp) of an ideal gas of linear and nonlinear molecules, chemical equilibrium. Mono atomic Crystals - Einstein and Debye models. T^3 dependence of heat capacity of solids at low temperatures. Numerical calculations of thermodynamic quantities for monoatomic, diatomic and polyatomic molecules.

Lecture 14, Marks 15

Recommended Books

1. Quantum Chemistry – Ira N. Levine, Pentice Hall
2. Statistical Mechanics – D.A. McQuarrie, Viva Books.
3. Physical Chemistry – P.W. Atkins, Oxford University Press.

Further Reading

1. Introduction to Quantum Chemistry – A.K. Chandra, Tata McGraw Hill.
2. Molecular Quantum Mechanics – P.W. Atkins & R.S. Friedman, Oxford University Press.
3. QuantumChemistry –D.A. McQuarrie, VivaBooksPvt.Ltd.:New Delhi
4. Chemical Kinetics – K. J. Laidler, Pearson Education India.
5. Physical Chemistry of Surfaces – A. W. Adamson, Wiley India Pvt. Ltd.
6. An Introduction to Statistical Thermodynamics – T.L. Hill, Dover Books.
7. Statistical Thermodynamics – M.C. Gupta, Wiley Eastern Ltd.
8. Statistical Mechanics and its Chemical Applications – M. H. Everdell Academic Press.
9. Statistical Thermodynamics – B.J. McClelland, Chapman and Hall Ltd.
10. Fundamental of Statistical Thermodynamic – R.E. Sontagg& Gordon J.V.

SEMESTER II

Title of the Course: Organic Chemistry Laboratory
Course Code: PCHC-204
Total Credits: 6
Distribution of Marks: 150 (End Sem 90 + Internal Assessment 60)

Course Objective: This core laboratory course in organic chemistry introduces students to common organic chemistry laboratory practices, techniques for carrying out and monitoring a synthesis, and quantitative estimation/characterization of organic compounds.

Learning Outcome: From this course, the students will understand organic chemistry from experimental point of view enabling them to perform qualitative analysis of organic compounds and mixtures.

A.

1. Organic Estimation - i) Estimation of glucose and sucrose in a mixture.

ii) Estimation of acetone by iodoform method.

iii) Estimation of hydroxyl and amino groups by acetylation method.

2. Separation and identification of three components of organic compounds present in a mixture by TLC.

Marks 25

Viva 5

B. 1. Separation and identification of amino acids present in a mixture by paper chromatography.

2. Organic Preparation - One –step preparation

i) Cannizaro reaction of benzaldehyde (separation of benzyl alcohol and benzoic acid by solvent extraction)

ii) Oxidation of p-nitrotoluene to p-nitrobenzoic acid

iii) Reduction of benzophenone to benzhydrol

iv) Phthalic anhydride to phthalimide

Marks 25

Viva 5

C. Preparation, purification (by TLC) and spectroscopic identification (UV and IR) of the prepared organic compounds and (B) Estimation]

Preparation: i. Benzilic acid from benzoin via benzyl (Benzilic acid rearrangement)

ii. Benzanilide from benzophenone via oxime (Beckman rearrangement)

iii. Indigo from anthranilic acid via phenylglycine-o-carboxylic acid and indoxyl

iv. Sandmeyer reaction- (a) ortho-Chlorotoluene from ortho-toluidine (steam distillation of the product)

(b) Acridone from anthranilic acid via o-chlorobenzoic acid and N-phenylanthranilic acid

v. Sulphanilamide from acetanilide via p-acetamidobenzenesulphonylchloride and p-acetamidobenzenesulphonamide

vi. Pinacolone from benzophenone via pinacol (Pinacolpinacolone rearrangement)

Marks 25

Viva 5

Recommended Books:

1. Furniss, B. S.; Hannaford, A. J.; Smith, P. W. G.; Tatchell, A. R., Vogel's Textbook of Practical Organic Chemistry, 5th Ed., Pearson Education India, New Delhi (2003).

2. Mann, F. G.; Saunders, B. C., Practical Organic Chemistry, 4th Ed., Pearson Education India, New Delhi (2009).

3. Clarke, H. T., A Handbook of Organic Analysis: Qualitative and Quantitative, 4th Ed., CBS Publishers, New Delhi (2007).

SEMESTER III

Title of the Course: Inorganic Chemistry
Course Code: PCHC-301
Total Credits: 4
Distribution of Marks: 100 (End Sem 60 + Internal Assessment 40)

Course Objective: This course on inorganic chemistry, will give a brief knowledge on group theory, inorganic spectroscopy and inorganic photochemical reaction.

Learning Outcome: Students will understand importance of group theory and applications in chemical science, will able to solve spectroscopic problems for Inorganic molecules.

UNIT I: A. Symmetry operation, elements of symmetry

Matrices and matrix representation of symmetry operations, Definition of Group, finite and infinite group. Examples of groups using geometrical object and symmetry operations. Symmetry elements as elements of group. Point groups. Orthogonality theorem: reducible and irreducible representation, use of vectors and mathematical functions in group representation, Character table for molecular point group, construction of C2v and C3v Character table. Direct product representation. Projection operator, symmetry adapted linear combination (SALC) for C2v, C3v, D 4h and Td point group molecules.

B. Chemical Application of Group Theory

Use of group theory in construction of hybrid Orbitals (d^2sp and sp^3 hybrids). Infrared absorption and Raman scattering spectroscopy, vibrational modes as bases for group representation, Symmetry selection rules for IR and Raman Spectra. Classification of vibrational modes and vibrational analysis. Orbital Symmetry and Chemical reactions – Woodward and Hoffman rules for electrocyclic and cycloaddition reactions.

Lecture 25, Marks 25

Unit II A. Application of NMR spectroscopy (^1H, ^{31}P and ^{19}F): Chemical shift, factors contributing to chemical shift, spin-spin coupling and its implication to structure determination; simplification of complex spectra; Use of 31P and 19F NMR incoordination chemistry: metal-ligand interaction; isomer determination; evaluation of stereo chemical non-rigidity in molecules; NMR spectra of paramagnetic compounds.

Marks 6

B. NQR spectroscopy: Principle of NQR, Quadruple constant, Application of NQR spectroscopy.

Marks 3

C. ESR spectroscopy: Principle, resonance condition, Origin of g-value, spin orbit coupling, Kramer degeneracy, zero-field splitting, hyperfine &superhyper interaction, line width and application of ESR in organic radicals and transition metal coordination complexes (e.g., d^1, d^3 and d^9).

Marks 6

D. Mossbauer spectroscopy: Principle of Mossbauer spectroscopy, Instrumentation, Application of Mossbauer spectroscopy: the isomer shift, magnetic interaction, quadruple splitting, line with. Application to iron to iron and tin compounds.

Marks 5

Lecture 20, Marks 20

UNIT III: Photochemical Reactions

Introduction to Inorganic Photochemistry, photophysical and photochemical processes, characteristics of the electronically excited states of inorganic compounds–ligand field states, charge transfer states, Frank-Condon, and thexi states, kinetics of photochemical process. Photochemical reactions: substitution and redox reactions of chromium, cobalt and ruthenium complexes. Relevance of ruthenium polypyridine complexes in solar energy conversion and storage, photo splitting of water, Inorganic photochemistry in biological processes and their model studies.

Lecture 15, Marks 15

Recommended Books

1. Cotton, F. A., Chemical Applications of Group Theory, 3rd Ed., Wiley India, New Delhi (2008).
2. Reddy, K. V., Symmetry and Spectroscopy of Molecules, 2nd Ed., New Age International Publishers, New Delhi (2009).
3. Housecroft, C. E; Sharpe, A. G., Inorganic Chemistry, 5th Ed., Pearson Education, Essex (2018).
4. Atkins, P.; Overton, T.; Rouke, J.; Weller, M.; Armstrong, F.; Hagerman, M., Shriver Atkins’s Inorganic Chemistry, 6th Ed., Oxford University Press, New Delhi (2015).
5. Miessler, G.; Tarr, D. A., Inorganic Chemistry, 3rd Ed., Pearson Education India, New Delhi (2008).

6. Huheey, J. E.; Keiter, E. A.; Keiter, R. L.; Medhi, O. K., Inorganic Chemistry: Principles of Structures and Reactivity, 4th Ed., Pearson Education India, New Delhi (2006).
7. Lampman, G. M.; Pavia, D. L.; Kriz, G. S.; Vyvyan, J.R., Introduction to Spectroscopy, 5th Ed., Cengage Learning India, New Delhi (2015).
8. Sathyanarayana, D. N. Handbook of Molecular Spectroscopy, 2nd Ed., IK International Publishing, New Delhi (2019).
9. Silverstein, R. M.; Webster, F. X.; Kiemle, D. J.; Bryce, D. L., Spectrometric Identification of Organic Compounds, 8th Ed., Wiley India, New Delhi (2015).
10. Kemp, W., Organic Spectroscopy, 3rd Ed., Macmillan Publishers India, New Delhi (2011).

Further Reading

1. Carter, R. L., Symmetry and Group Theory, Wiley India, New Delhi (2009).
2. Jordan, R. B.; Reaction Mechanisms of Inorganic and Organometallic Systems, 3rd Ed., Oxford University Press, New York (2007).
3. Roundhill, D. M., Photochemistry and Photophysics of Metal Complexes, Plenum: New York (1994).
4. Basolo, F.; Pearson, R. G., Mechanisms of Inorganic Reactions: Study of Metal Complexes in Solution, 2nd Ed., John Wiley and Sons, New Jersey (1975).

SEMESTER III

Title of the Course: Organic Chemistry-III
Course Code: PCHC-302
Total Credits: 4
Distribution of Marks: 100 (End Sem 60 + Internal Assessment 40)

Course objective: This course will enable the students to comprehend various types of organic reactions, their mechanisms and applications.

Learning outcome: Through this course students will acquire the detailed knowledge on substitution, elimination, addition, oxidation and reduction, photochemical and pericyclic reactions.

UNIT I: Oxidation

(i) of carbon-carbon double bond: dihydroxylation by $KMnO_4$, OsO4 (including Sharpless asymmetric dihydroxylation), iodine and silver carboxylate (Woodward and Prevost condition) and peroxy acid. Allylic and benzylic oxidation of alkene: Use of SeO2 and DDQ.
(ii) of alcohols: Use of Cr(VI) based reagents (PCC, PDC), DMSO-based reagents (Swern, Pfitzner-Moffatt and Albright – Goldman), Tetrapropyl ammonium perruthenate (TPAP); (iii) of 1,2- diols.

Lecture 12, Marks 12

UNIT II: **Reduction**

(i) by catalytic hydrogenation: both heterogeneous (H2 /Pd-C, H2 /Pt2O, Lindlar's and Rosendmund's reduction) and homogeneous (Wilkinson catalyst),
(ii) by modified hydride transfer reagents (Lithium trialkoxyaluminium hydrides, DIBAL, NaCNBH4 , SMEAH (Red Al), Superhydride and Selectrides, 9-BBN
(iii) by dissolving metal (alkali metals in liquid ammonia) and
(iv) by diimide. Electrooxidation and reduction, Use of Baker's Yeast.

Lecture 12, Marks 12

UNIT III: Substitution, Elimination and Addition Reactions Substitution Reactions: Mechanism and reactivity of aromatic, aliphatic, nucleophilic substitution reaction, orientation and reactivity in aromatic electrophillic substitution reactions. Elimination Reactions: Mechanism, orientation and reactivity, dehydration of alcohols, Shapiro reaction, conversion of epoxide to olefins, dehalogenation of vicinal halide. Substitution vs.

elimination, nucleophile vs. base. Addition Reactions: Mechanism and stereochemical aspects of addition reactions in carbon-carbon multiple bonds.

Lecture 12, Marks 12

UNIT IV: Photo organic and Pericyclic Reactions Photo organic Chemistry:

Photoorganic Chemistry: cis-trans isomerisation, Norrish type I & II reaction, photoreduction of ketones, Paterno-Buchi reaction, Di- π-methane and Di-π-methane type rearrangement. Introduction, types: electrocyclic, cycloaddition and sigmatotropic reaction; 1,3-dipolar addition, Ene reaction, selection rules, general orbital symmetry rules.

UNIT V: **Heterocyclic Chemistry**

Small Ring Heterocycles: Syntheses of aziranes, oxiranes & thiiranes; ring openings and heteroatom extrusion; synthesis & reactions of azetidines, oxetanes & thietanes. Aromatic heterocycles: Synthesis and reactions of furan, thiophene, pyrrole, pyridine, quinoline, isoquinoline and indole. Concept of π-excessive and π-deficient heterocyclics. Condensed Five-membered Rings (1 Heteroatom): Synthesis and reactions of indole, benzofuran and benzothiophene. Diazines: Structural & chemical properties; Synthesis of pyridazines, pyrimidines, pyrazines, nucleophilic and electrophilic substitutions.

Lecture 12, Marks 12

Recommended Text Books

1. Smith, M. B.; March, J., March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 7th Ed., Wiley India, New Delhi (2015).
2. Smith, M. B., Organic Synthesis, 4th Ed., Academic Press, Cambridge, Massachusetts (2016).
3. Greeves, N.; Clayden, J.; Warren, S., Organic Chemistry, 2nd Ed., Oxford University Press, New Delhi (2012).

Further Reading

1. Carruthers, W., Modern Methods of Organic Synthesis, 4th Ed., Cambridge University Press, New Delhi (2005).
2. Zweifel, G. S.; Nantz, M. H.; Somfai, P., Modern Organic Synthesis: An Introduction, 2nd Ed., Wiley-Blackwell, New York (2017)

SEMESTER III

Title of the Course: Physical Chemistry-III
Course Code: PCHC-303
Total Credits: 4
Distribution of Marks: 100 (End Sem 60 + Internal Assessment 40)

Course objective: This course impart knowledge on theories of reaction kinetics, applications of electrochemistry and the structure and symmetry of crystalline solids, its defects and applications of band theory.

Learning outcome: Through this course students will acquire the detailed knowledge on the theories of reaction kinetics and will be able to solve problems related to different types of reaction kinetics and catalysis. Students will understand the concepts electrochemistry, properties and applications solids.

UNIT I: Chemical Kinetics and Reaction Dynamics

Methods of determining rate laws, Activated complex theory, structure of transition state, Eyring equation, chain reactions and oscillatory reaction, steady state approximation. Unimolecular reactions – Drawbacks of Lindemann theory, Hinshelwood, Kassel, Rice and Ramsperger theory, Stater's Theory. Relaxation kinetics – linearized rate equation, relaxation time (in single step reaction) ; determination of relaxation time and rate constant, Methods of studying fast reaction – flow method, temperature jump and pressure jump method, NMR method, flash photolysis. Reactions in solution – Factors determining reaction rates in solution, reactions involving ion-ion and ion-dipoles reaction; influence of solvent, ionic strength and pressure on the reactions in solution. Rate of enzyme catalyst reaction, Michaelis-Menten equation; temperature, pH and concentration dependence of enzyme catalysed reactions; acid-base catalysis and acidity function. Kinetics of polymerization.

Lecture 22, Marks 30

UNIT II: **Electrochemistry**

General electrochemical concepts. Introduction to electrochemistry: thermodynamics, electrode potentials, galvanic and electrolytic cells, electrode kinetics, dynamic electrochemistry, mass transport by migration, diffusion and convection, diffusion layers. Ion-Solvent Interaction: Ion-Dipole, Ion-quadruple, Ion-Induced Dipole Interaction, Ion-Association: Bjerrums hypothesis, Thermodynamics of ion-pairing, relation between Debye-Huckel free ion and Bjerrums ion-pair. Polarizable and non polarizable electrodes. Inner and

Outer potential, Thermodynamics of Electrified Interfaces: Surface Excess and its determination. Electrical double layer (DL): HP/ GC/ Stern model. Potential variation in DL and capacity of DL.

Lecture 14, Marks 15

UNIT III: Solid State Chemistry

Crystal Systems, Brief description of crystal symmetry and point group (Hermann Mauguin symbols), Space group (Monoclinic and Triclinic systems). Crystal defects (Frenkel and Schottky), line (edge and screw dislocations) and plane defects (grain boundaries and staking fault), Octahedral and tetrahedral voids. Electronic structure: Band theory of solids, electrical and magnetic properties of solids.

Lecture 14, Marks 15

Recommended Text Books

1. Chemical Kinetics – K. J. Laidler, Pearson Education India.
2. Modern Electrochemistry – Vol I, II by J. O. M. Bockris & A. K. N. Reddy
3. Solid State Chemistry and its Application – A. R. West, Wiley India.

Further Reading

1. Chemical Kinetics and Reaction Dynamics – P. L. Houston, Dover Publications
2. Kinetics and Mechanism – A. A. Pearson, R. G. Frost, John Wiley and Sons
3. Electrochemical Methods: Fundamentals and Applications, A. J. Bard, L. R. Faulkner, John Wiley and Sons.
4. An Introduction to Electrochemistry – S. Glasstone, East West Press.
5. Physical Chemistry – P.W. Atkins, Oxford University Press.
6. Solid State Chemistry – D. K. Chakravorty
7. Principles of Solid State – H. V. Keer, New Age International.

SEMESTER III

Title of the Course: Physical Chemistry Laboratory
Course Code: PCHC-304
Total Credits: 6
Distribution of Marks: 150 (End Sem 90 + Internal Assessment 60)

Course Objective: This core laboratory course introduces students to experimental physical chemistry involved with basic physical chemistry such as chemical kinetics, surface chemistry, thermodynamics, spectrophotometry etc.

Learning Outcome: From this course, the students will understand physical chemistry from experimental point of view.

A.

1. To determine the rate constant of hydrolysis of methyl acetate catalyzed by an acid and also the energy of activation.
2. To determine the velocity constant of hydrolysis of ethyl acetate by NaOH.
3. Determine the rate constant of inversion of cane sugar by analytical method.
4. Study the kinetics of the reaction between iodine and acetone in acidic medium by half-life period method and determine the order with respect to iodine and acetone.
5. Determine the molar mass of a polymer by viscometric method.

Marks 25

Viva 5

B.

1. To study hydrolysis of methyl acetate in presence of HCl and H2SO4 and hence determine the relative strength of the acids(use Guggenheim method) i) analytically. ii) polarimetrically.
2. Determine the equivalent conductivity of acetic acid at infinite dilution by Kohlrausch's method.
3. Determine the relative strength of acetic acid and monochloro acetic acid by conductance measurement.
4. Determine the specific rotation of sucrose and hence determine the unknown concentration of supplied solution by polarimetric measurements.
5. Determination of pH of a mixture of CH3COOH and CH3COONa, and hence determine the dissociation constant of the acid. 6. Preparation of conducting polymers and study of their electrical conductivity.

Marks 25

Viva 5

C.

1. Determination of hydrolysis constant of aniline hydrochloride by pH measurements.
2. Determine the strengths of the components of the following mixtures by conductometric titration a) Hydrochloric acid and acetic acid b) Sulphuric acid and copper sulphate
3. Determine the strengths of HCl and CH3COOH in a given mixtures by pH-metric titration.
4. Verify Beer's law and determine the unknown concentration of supplied solutions like KMnO4 / K2Cr2O7
5. Determine the composition of iron-salicylic acid complex spectrophotometrically by Job's method.
6. Least squares fitting and plotting linear and exponential graphs performing theoretical calculations using a computer

Marks 25

Viva 5

Recommended Books:

1. Halpern, A. M.; McBane, G. C., Experimental Physical Chemistry: A Laboratory Textbook, W. H. Freeman, New York (2006).
2. Viswanathan, B.; Raghavan, P. S., Practical Physical Chemistry, Viva Books, New Delhi (2014).
3. Yadav, J. B., Advanced Practical Physical Chemistry, Krishna Prakashan, Meerut (2015).

SEMESTER IV

Title of the Course: Inorganic Chemistry-IV
Course Code: PCHC-401
Total Credits: 4
Distribution of Marks: 100 (End Sem 60 + Internal Assessment 40)

Course Objective: In this course on inorganic chemistry, will provide a thorough knowledge about Inorganic reaction mechanism, Organometallic Chemistry and various catalytic processes, both homogeneous and heterogeneous systems.

Learning Outcome: Students will gain advanced knowledge on various types of organometallic complexes and their utility as catalysts in various organic reactions.

UNIT I: Introduction to transition metal organometallic chemistry: Metal carbon bond formation,18 and 16 electron organometallic complexes. Isolobel analogy in organometallic compounds. Bonding in organo-transition metal compounds: Metal carbonyls, metal olefins, metal carbene, Role of CO-ligands like phosphine, arsine, stibine, N_2, O_2 and NO. Oxidative addition, reductive elimination and β-elimination reaction.

Lecture 8, Marks 8

UNIT II: Organo-transition metal Chemistry: Structure and bonding of pi bonded organometallic compounds including carbonyls, nitrosyls, tertiary phosphines, hydrides, alkene, alkyne, cyclobutadiene, cyclopentadiene, arene compounds. Metal-carbon multiple bonds. Fluxional organometallic compounds including π-allyl complexes. Carbon σ donors: Synthesis of metal alkyls and aryls, direct reaction of a metal with organic halides, reaction of anionic alkylating agents with metal halides, Metallation reactions.

Lecture 15, Marks 15

UNIT III: Homogeneous and Heterogeneous catalysis: Introduction and definition; alkene metathesis (olefins); alkene hydrogenation, carbonylation, hydroformylation, alkene oligomerization, polymerization, polymer supported and biphasic catalysis, transition metal organometallic clusters, surfaces and interactions with adsorbates, Fischer-Tropsch carbon chain growth; use of ZSM-5 for organic transformations; Suzuki-Miyaura, Heck and Sonogashira cross-coupling reactions. Activation of small molecules (O_2, H_2, N_2, CO and CO_2).

Lecture 15, Marks 15

UNIT IV: Electron transfer reaction: Rearrangement of Precursor complex and electron transfer; Nature of bridging ligand;2-electron transfer; Synthesis of coordination compounds using redox reaction; complementary and non-complementary reaction; Oscillating reactions; Template effect and macrocyclic ligands; reactions of coordinated ligands. Synthesis of coordination compound by substitution reactions; Isomerization and racemization of tris-chelate complexes; Molecular rearrangement in four-coordinated and six-coordinated complex.

Lecture 10, Marks 12

Recommended Books

1. Housecroft, C. E; Sharpe, A. G., Inorganic Chemistry, 5th Ed., Pearson Education, Essex (2018).
2. Atkins, P.; Overton, T.; Rouke, J.; Weller, M.; Armstrong, F.; Hagerman, M., Shriver Atkins's Inorganic Chemistry, 6th Ed., Oxford University Press, New Delhi (2015).
3. Miessler, G.; Tarr, D. A., Inorganic Chemistry, 3rd Ed., Pearson Education India, New Delhi (2008).
4. Huheey, J. E.; Keiter, E. A.; Keiter, R. L.; Medhi, O. K., Inorganic Chemistry: Principles of Structures and Reactivity, 4th Ed., Pearson Education India, New Delhi (2006).

Further Reading

1. Cotton, F. A.; Bochmann, M.; Murillo, C. A.; Wilkinson, G., Advanced Inorganic Chemistry, 6th Ed., Wiley India, New Delhi (2007).
2. Figgis, B. N.; Hitchman, M. A., Introduction to Ligand Field Theory and Its Applications, Wiley India, New Delhi (2010).

SEMESTER IV

Title of the Course: Inorganic Chemistry-V
Course Code: PCHC-402
Total Credits: 4
Distribution of Marks: 100 (End Sem 60 + Internal Assessment 40)

Course Objective: In this course on inorganic chemistry, will provide general knowledge about nuclear chemistry, cluster chemistry, Supramolecular Chemistry and advance knowledge on the area of nanomaterials.

Learning Outcome: Students will learn the depth of Inorganic Chemistry in a more holistic way so that they can compete for various type of competitive examinations.

UNIT I: Clusters

Definition of clusters, Low and high nuclearity metal carbonyl and metal halide clusters, bimetallic clusters. Closed shell electronic requirements for cluster compounds, introduction to tensor surface harmonic theory of clusters. Organization of neutral boron hydrides, anionic borane, carboranes and metallocarboranes. Synthesis and properties of C60.

Lecture 10, Marks 12

UNIT II: Nuclear Chemistry Nuclear structure and nuclear stability, Radioactivity and Nuclear reactions, fission and fusion, radio-analytical techniques and activation analysis.

Lecture 8, Marks 10

UNIT III: Supramolecular Chemistry: Origin of supramolecular chemistry. Concepts and terminology of supramolecular chemistry. Types of supramolecular interactions (Hydrogen bonding, van der Waals interaction, π-stacking, CH-π, anion-π interaction). Host-guest Chemistry: macrocyclic effect and their thermodynamic origin, Step-wise and overall binding constant in host-guest chemistry, kinetic and thermodynamic selectivity. Binding of organic and inorganic cationic, anionic, ion pair and neutral guest molecules with host molecules. Molecular recognition,Supramolecular reactivity and catalysis, Effects of medium, Chiral recognition. Self-assembly: Definitions and basic concepts of self-assembly, self-assembly using metal templates. Applications of self-assembled molecules.

Lecture 12, Marks 12

UNIT IV: Materials Chemistry

A. Synthesis and modification of inorganic solids: General principle of solid state reaction, experimental procedure (coprecipitation, Sol-gel, Hydrothermal, Intercalation etc.), Preparation of crystalline materials, nucleation, crystal growth, Graphite and zirconium intercalation compounds, transition metal chalcogenide, thin films, growth of single crystals. Catalyst immobilization onto silica and clay surfaces and applications, pillaring of certain clays. Electronic and optical properties of some inorganic and organic solids (Solid electrolytes, Inorganic coloured solids, white and black pigments). Design and properties of composites, polymer matrix and carbon-carbon composites. Brief idea about drilling muds.

Marks 18

B. Introduction to physics and Chemistry of solid materials, energy bands: conductor, semiconductor and insulator; Graphite, graphene-oxide, diamond. Size and morphology dependence properties. Methods of measuring properties: crystallography, size of particles, surface structure. Synthesis and Properties of nanomaterials: Metal oxide, semiconducting nanoparticles. Nanoclusters, Composites and Nanotubes. Top-Down and Bottom-Up approach, Quantum confinement effect and Surface plasmon resonance. Application of various solid materials in fuel cell, photovoltaic cell, in electrochemistry as electrode materials (capacitor material), photocatalysis and chemical sensors.

Marks 18.

Lecture 30, Marks 26

Recommended Books

1. Housecroft, C. E; Sharpe, A. G., Inorganic Chemistry, 5th Ed., Pearson Education, Essex (2018).
2. Atkins, P.; Overton, T.; Rouke, J.; Weller, M.; Armstrong, F.; Hagerman, M., Shriver Atkins’s Inorganic Chemistry, 6th Ed., Oxford University Press, New Delhi (2015).
3. Miessler, G.; Tarr, D. A., Inorganic Chemistry, 3rd Ed., Pearson Education India, New Delhi (2008).
4. Huheey, J. E.; Keiter, E. A.; Keiter, R. L.; Medhi, O. K., Inorganic Chemistry: Principles of Structures and Reactivity, 4th Ed., Pearson Education India, New Delhi (2006).
5. Steed, J. W.; Turner, D., R.; Wallace, K. J., Core Concepts in Supramolecular Chemistry and Nanochemistry, John Wiley & Sons, West Sussex (2007).

6. Steed, J. W.; Atwood, J. L., Supramolecular Chemistry, 2nd Ed., John Wiley & Sons, West Sussex (2009).
7. West, A. R., Solid State Chemistry and its Application, Wiley India, New Delhi (2007).
8. Smart, L. E.; Moore, E. A., Solid State Chemistry: An Introduction, 4 th Ed., CRC Press, New Delhi (2017).
9. Kakani, S. L.; Kakani, A., Material Science, 3 rd Ed., New Age International Publishers, New Delhi (2016).
10. Skoog, D. A.; Holler, F. J.; Crouch, S. R., Principles of Instrumental Analysis, 6th Ed., Cengage Learning India, New Delhi (2014).
11. Poole, C. P. Jr.; Owens, F. J., Introduction to Nanotechnology, Wiley India, New Delhi (2007).
12. Pradeep, T., Nano: The Essentials-Understanding Nanoscience & Nanotechnology, Tata McGraw Hill India, New Delhi (2017).

Further Reading

1. Cotton, F. A.; Bochmann, M.; Murillo, C. A.; Wilkinson, G., Advanced Inorganic Chemistry, 6th Ed., Wiley India, New Delhi (2007).
2. Ariga, K.; Kunitake, T., Supramolecular Chemistry: Fundamentals and Applications, Springer, Heidelberg (2006).
3. Rao, C. N. R.; Gopalakrishnan, J., New Direction in Solid State Chemistry, 2nd Ed., Cambridge University Press, Cambridge (1997).
4. Keer, H. V., Principles of the Solid State, 2nd Ed., New Age International Publishers, New Delhi (2017).
5. Lehn, J.-M., Supramolecular Chemistry: Concepts and Perspectives, Wiley India, New Delhi (2014).

SEMESTER IV

Title of the Course: Organic Chemistry-IV
Course Code: PCHC-403
Total Credits: 4
Distribution of Marks: 100 (End Sem 60 + Internal Assessment 40)

Course objective: This course will enable the students to comprehend the basics of retrosynthesis and its importance in planning an organic synthesis, important reagents and methods of organic synthesis.

Learning outcome: Through this course students will acquire the detailed knowledge on planning of synthesis of complex organic molecules and about reagents and methods to achieve targeted synthetic molecules.

UNIT I: Disconnection approach in organic synthesis:

Acceptor and donor synthons, Use of umpolung, Retrosynthesis of Alcohols (Grignard approaches and hydride transfer approaches) and Carbonyl compounds. One group and two group C-X disconnections. One group and two group C-C disconnections. Retrosynthsis of 1,2-, 1,3-, 1,4-, 1,5- and 1,6- difunctional (O,O and N,O in a difunctional relation) compounds. Use of protecting groups in organic synthesis: protection and deprotection of hydroxyl, dihydroxy, carbonyl, carboxyl and amino groups.

Lecture 14, Marks 14

UNIT II: **Advanced Stereochemistry**

Conformational analysis of disubstituted cyclohexanes, cyclohexene, cyclohexanone, 2-alkyl, 3-alkyl, and 4-alkyl ketone effects. A 1,2 and A 1,3 strains. Conformation of fused systems - decalins and perhydrophenanthrenes. Effects of conformation on reactivity and mechanism of basic organic reactions of 6-membered ring compounds. Chiroptical properties - Optical rotatory dispersion, circular birefringence, circular dichroism, axial haloketone rule, octane rule.

Lecture 12, Marks 12

Unit III Study of the following reactions, their mechanism and synthetic utility

Metal mediated C-N coupling reactions: Buchwald-Hartwig, Ullmann and Chan-Lam cross-coupling reactions; Henry reaction, Mitsunobu reaction, Corey-Nicolaoumacro lactonization,

Baylis Hilman reaction, Vilsmeier– Haack reaction, Wohl Ziegler allylic bromination, Barton reaction.

Lecture 12, Marks 12

UNIT IV: Elementary idea of PASE synthesis, Combinatorial Chemistry, Parallel synthesis, Microwave synthesis.Nanocatalysis in Organic synthesis.Olefin metathesis.

Lecture 10, Marks 10

UNIT V: **Reagents in Organic Synthesis**

9-BBN, IBX, Dess-Martin periodinane, Fetizon reagent, dioxiranes, Gilman's reagent, lithium disopropylamide, dicyclohexylcarbodimide, 1,3-dithiane reactivity: Umpolung effect, Phase transfer catalyst, Tebbe reagent, Baker's yeast, NBS, Mosher's reagent, DDQ.

Lecture 12, Marks 12

Recommended Books

1. Warren, S., Organic Synthesis: The Disconnection Approach, Wiley India, New Delhi (2007).
2. Nasipuri, D. Stereochemistry of Organic Compounds: Principles and Applications, 3rd Ed., New Age International Publishers, New Delhi (2018).
3. Carruthers, W., Modern Methods of Organic Synthesis, 4th Ed., Cambridge University Press, New Delhi (2005).

Further Reading

1. Smith, M. B., Organic Synthesis, 4th Ed., Academic Press, Cambridge, Massachusetts (2016).
2. Kurti, L., Czako, B., Strategic Application of Named Reactions in Organic Synthesis, Elsevier, Amsterdam (2005)

SEMESTER IV

Title of the Course: Organic Chemistry-IV
Course Code: PCHC-404
Total Credits: 4
Distribution of Marks: 100 (End Sem 60 + Internal Assessment 40)

Course objective: This course will impart knowledge on action of various drugs, QSAR concept and interaction mechanism, also basic knowledge on petroleum technology.

Learning outcome: Through this course students will acquire the detailed knowledge on action of different drugs, factors affecting their bioactivity and mode of action and also understand the basics of petroleum industry.

UNIT I: Drugs

Definition of drugs and factors affecting their bioactivity; Definition of chemotherapeutic index and therapeutic index. Quantitative structure activity relationship (QSAR). Concepts of drug receptor, theoretical aspects of drug receptor interaction. Drug introduction, Metabolism, Excretion. Introduction to designing of drugs; Structural modification of drugs. Introduction to combinatorial library of drugs. Sulphadrugs: Historical significance of sulpha drugs as antibacterial agent, Sulphanilamide and other important sulpha drugs and their mode of action. Antibiotics : Introduction and classification, Structure action relationship and mode of action of penicillin, semisynthetic penicillins, streptomycin, tetracyclins. Antimalarials: Introduction and classification, human malaria and plasmodia, mepaquine, trimethopriim and mefloquine – their structure and activity as antimalarials. Artemisinin and its derivatives, structure-action relationship. Drugs used for treatment of cancer and tuberculosis and recent developments.

Lecture 18, Marks 18

UNIT II: **Organic synthesis I**

Organometallic reagents in formation of carbon-carbon bonds: Organopalladium in C-C formation (Heck reaction, Stille, Suzuki, Sonogashira and Negishi Coupling). Formation of C=C bonds by elimination reactions, syn elimination; Wittig and related reactions, McMurry reaction, Peterson olefination, Julia reaction and Tebbeolefination. Use of organosulphur compounds for reversal of polarity (Corey-SeebachUmpolung). Allylic activation by - allyl Ni and – allyl Pd complexes.

Lecture 14, Marks 14

Unit III Organic synthesis II

Application of Enamines, Hydroboration and trialkylsilyl halides in organic synthesis. Use of the following reagents: Organotin (TBTH), Lithium Diisopropyl Amide (LDA), Dicyclohexylcarbodiimide, Dicyanodichloroquinone (DDQ), Dimethyl dioxirane (DDO), lipase and other reagents of organozinc and organocopper.

Lecture 12, Marks 12

UNIT IV: **Petroleum Technology**

'Upstream'— the exploration and production sector of the industry; survey, exploration, drilling, drilling fluid, well stimulation, enhanced oil recovery, transportation and storage. 'Downstream'—the sector which deals with refining and processing of crude oil and gas products; petroleum product profile, crude oil evaluation, natural gas and petroleum products, processing and purifying/refining of crude oil and natural gas, reforming. Environmental management and corrosion prevention in petroleum technology.

Lecture 15, Marks 15

Recommended Text Books

1. Stereochemistry of Carbon Compounds – Earnest E. Eliel, Tata McGraw Hill
2. Stereochemistry of Carbon Compounds – Subrata Sengupta, New Central Book agency, Kolkata
3. Stereochemistry and Mechanism through Solved Problems- P.S. Kalsi, New Age International Publishers
4. Organic Synthesis – M.B. Smith, McGraw Hill. (Reference book)
5. Principles of Organic Synthesis – R.O.C. Norman and J M Coxon
6. Advanced Organic Chemistry Part A and B : Carey and Sundberg
7. Organic Synthesis – J. Singh and L.D.S.Yadav, PragatiPrakashan
8. Application of Redox and Reagents in Organic Synthesis- R.K. Kar, New Central Book Agency
9. Fundamentals of Organic Synthesis : The Retrosynthetic Analysis - R.K. Kar, NCBA
10. Synthetic Approaches in Organic Chemistry – R.K. Bansal- Narosa Publishing House, New Delhi
11. Modern Synthetic Reactions – H.O. House, W.A. Benjamin, NY
12. Oil and Gas Production Handbook: an Introduction to Oil and Gas Production, Transport, Refining and Petrochemical Devold Havard

13. The Organic Chemistry of Drug Design and Drug Action – Richard B.Silverman, Elsevier Science Publishing Co Inc

Further Reading

1. Stereochemistry of Organic Compounds – D. Nasipuri, Wiley Eastern
2. Modern Methods of Organic Synthesis – Carruthers and Coldham, Cambridge University Press
3. Fundamentals of Oil & Gas Industry for Beginners – Samir Dalvi, Notion Press

SEMESTER IV

Title of the Course: Physical Chemistry-IV
Course Code: PCHC-405
Total Credits: 4
Distribution of Marks: 100 (End Sem 60 + Internal Assessment 40)

Course objective: This course will enable the students to understand the concepts of dynamic electrochemistry, solid state electrochemistry, electrocapillary phenomenon, electrocatalysis and nanostructured and surface modified electrodes and impart knowledge on criteria and assumptions of non-equilibrium thermodynamics.

Learning outcome: Through this course students will gain knowledge in the thermodynamic and kinetic aspects of Electrochemistry through different fundamental concepts and models. Students will develop the skills to solve problems in non-equilibrium thermodynamics.

UNIT I: **Advanced Electrochemistry**

Introduction to electrochemistry: Nernst equation, electrode kinetics, dynamic electrochemistry, the Butler-Volmer and Tafel equations. Overpotentials. Kinetically and mass transport controlled electrochemical processes. Mass transport by migration, convection and diffusion. Conductivity. Solid state electrochemistry. Ion conducting and electronically conducting polymers. The electrochemical double layer. Potentiostatic and galvanostatic electrochemical methods including chronoamperometry, coulometry, cyclic voltammetry and impedance spectroscopy. Thermodynamics of Electrocapillary phenomenon; Surface excess, relevance of outer and surface potential to double layer (DL) studies, surface and inner potential difference. Capacity potential relations in electrode-electrolyte interface, Contact adsorption-its influence on capacity of interface, Capacitance hump. Electrocatalysis: Definitions, Electrocatalytic potential, effect of electric field on electrocatalysis, Nanostructured and surface modified electrodes. Introduction to batteries, fuel cells and electrochemical solar cells. Electrochemical processes of particular relevance to energy conversion.

Lecture 30, Marks 35

Unit II: Non-equilibrium Thermodynamics

Difference between equilibrium and non-equilibrium thermodynamics, Criteria of non-equilibrium thermodynamics; Assumptions of non-equilibrium thermodynamics, uncompensated heat and its relation to other thermodynamic functions, Fluxes and forces relation between these two quantities, Entropy production in heat transfer, mass transfer in flow of current, in mixing of gases, and in chemical reaction; The Phenomenological equations: The linear laws, The Onsagar relation, microscopic reversibility and Onsager reciprocity. Coupled reaction. Thermoelectric effects: Seebeck, Peltier and Thompson effect.

Lecture 20, Marks 25

Recommended Books:

1. Modern Electrochemistry: Vol II by J. O. M Bockris & A. K. N. Reddy
2. Non Equilibrium Thermodymacis: Principles and application – C. Kalidas & M.V. Sangaranarayanan

Further Reading

1. Electrochemical Methods: Fundamentals and Applications, A. J. Bard, L. R. Faulkner, John Wiley and Sons.
2. Inorganic Electrochemistry: Theory, Practice and Applications by Piero Zanello
3. Non Equilibrium Thermodynamics by de Groot, S. R. and P. Mazur
4. Introduction to Thermodynamics of Irreversible Processes by I. Prigogine

SEMESTER IV

Title of the Course: Physical Chemistry-IV
Course Code: PCHC-406
Total Credits: 4
Distribution of Marks: 100 (End Sem 60 + Internal Assessment 40)

Course objective: This course will introduce the Hartree Fock theory for treatment of atoms and molecules, Density Functional Theory through historical developments and basic theorem. It will make students to understand the applications of statistical thermodynamics on complex systems like classical liquids, phase transitions in lattice models etc. and impart basic understanding of different simulation techniques.

Learning outcome: Through this course students will gain understanding of the advanced electronic structure of atoms/molecules through quantum mechanical methods, and will develop the skills to solve problems using those concepts. Students will gain knowledge about modern day computational treatments of atoms and molecules and will understand applications of Density Functional Theory. Students will be able to apply the concepts of statistical thermodynamics to understand complex systems and solve problems related to those systems. Students will understand the theoretical background of different simulations techniques and there applicability to different problems.

UNIT I: Advanced Quantum Chemistry

Antisymmetry Principle; Hartree product, Slater determinant; Slater-Condon rules; Hartree Fock equations, Koopmans' and Brillouin's theorems, Roothaan equations, SCF procedure. Computational treatment of atoms and molecules: Representation of molecules,Gaussian basis sets. Introduction to Density functional Theory: Hohenberg-Kohn theorems; chemical concepts within the density functional theory.

Lecture 26, Marks 30

UNIT II: Advanced Statistical Mechanics

Classical Liquids Interparticle potentials, Configurational Partition functions, distributions, pair correlation function,radial distribution function, neutron scattering experiments, Virial equation, Meyer cluster diagrams. Phase Transitions in Lattice models Lattice gas, Ising Model, order parameter, Mean Field theory, Renormalization group theory. Computer Simulations Ensemble averages, ergodicity, random numbers, Monte Carlo methods, Molecular Dynamics, constant temperature MD.

Lecture 24, Marks 30

Recommended Books:

1. Modern Quantum Theory – N. S. Ostlund and A. Szabo, McGraw Hill.
2. Statistical Mechanics – D.A. McQuarrie, Viva Books.

Further Reading:

1. Methods of Molecular Quantum mechanics, R. McWeeney and B. T. Sutcliffe, Academic Press.
2. Density functional theory of atoms and molecules, R. G. Parr and W. Yang, Oxford.
3. Introduction to Computational Chemistry by Frank Jensen
4. Essentials of Computational Chemistry: Theories and Models by C. J. Cramer
5. Molecular Modeling: Principles and Applications by A. R. Leach
6. An Introduction to Statistical Thermodynamics – T.L. Hill, Dover Books.
7. Statistical Mechanics – K. Huang, Wiley. 8. Statistical Thermodynamics – M.C. Gupta, Wiley Eastern Ltd.

SEMESTER IV

Title of the Course: Project Dissertation
Course Code: PCHC-407
Total Credits: 4
Distribution of Marks: 200 (End Sem 120 + Internal Assessment 80)

Course objective: The purpose of offering project work to the students is to encourage the students in research and innovation in frontier areas of chemistry. Through this course they would be introduced to various stages of research planning and implementation. Students will perform scientific research under the supervision of a faculty and learn to work independently. During the course of her/his project work, students are expected to learn different synthetic methods and analytical techniques for carrying out scientific research problems, particularly to collect and interpret data.

Learning outcome: Following the completion of this course, students should be able demonstrate ability to plan and strategize a scientific research problem, and implement it within a reasonable time frame. It is expected that after completing this project dissertation, students will learn to work independently and how to keep accurate/readable record of their experimental work. In addition, students will be able to handle laboratory equipment and chemicals. Also, students will be able to utilize sophisticated instruments for analysis, data collection and interpretation. Subsequently, the students should be able to critically examine research articles, and improve their scientific writing/communication skills

1. Research project approved by the Supervisor, preparation of the dissertation and presentation of the results and viva-voce examination by a board of examiners. Dissertation

Marks 90 Viva-Voce Marks 30