Course No: CH24201CR
Title: Inorganic Chemistry (04 Credits)

Max. Marks: 100 **Duration: 64 Contact hours**
Continuous Assessment: 20 marks **End Term Exam: 80 Marks**

Course outcomes:

- The course deals in detail with learning of inorganic reaction mechanism, which is generally not taught in good detail at the undergraduate level.
- Understanding of reaction rates and their dependence on various possible factors, like nature of incoming reagent, intermediates, orbital symmetry and ligands of the substrate.
- Prediction of rates of reaction.
- Differentiation between kinetic and thermodynamic controls of a reaction and identification of kinetic and thermodynamic products formed during reactions.
- Understanding of basic concepts, structure and applications of organo-metallic compounds.

Unit-I Mechanism of Ligand Substitution Reactions in Square-Planar complexes

(16 Contact hours)

Importance and need to study inorganic reaction mechanism. Energy profile of reactions, reaction intermediates and transition states. Reaction mechanism of square planar complexes, KS and KY pathways, nature of reaction intermediates/ transition states. ***(05 hrs)***

Factors affecting reactivity of square planar complexes: Nature of entering group-Nucleophilicity and basicity, nucleophilic constants n_{pt} and n_{Pt}^{o} scales. Trans-effect: Trans influence, theories and application in synthesis, Cis-Effect, nature of leaving group and central metal atom/ion. ***(09 hrs)***

Reactivity of metal complexes-Kinetic and thermodynamic stability, Identification inert and labile complexes. ***(02 hrs)***

Unit-II Mechanism of Ligand Substitution Reactions in Octahedral Metal Complexes

(16 Contact hours)

Mechanistic classification of substitution reactions: - Dissociative, Associative, and Interchange mechanism. Empirical criteria to differentiate the mechanism of substitution reaction. (**2 hrs**)

Replacement of coordinated water: Eigen-Wilkins Mechanism, Rates of water replacement. Classification of metal ions based on water exchange rates. LFAE considerations. Anation reactions. (**5 hrs**)

Base hydrolysis: Mechanistic details. Conjugate base (CB) mechanism, Rate of base hydrolysis. Case studies of base hydrolysis: effect of base concentration, nucleophiles, ligands with acidic protons and reactant isomerism. (**4 hrs**)

Acid hydrolysis: Mechanism, case studies of complexes without π-donar/acceptor ligands, with π-acceptor ligands and iii) with π-donor ligands. (**5 hrs**)

Unit-III Mechanism of Electron Transfer Reactions in Coordination Complexes

(16 Contact hours)

Classification of oxidation-reduction reactions: stoichiometric and mechanistic. inner sphere electron transfer reaction mechanism: taube reaction. elementary steps, precursor and successor complexes. bridging ligand effects, case of multidentate ligands, electron transfer through extended bridges, double bridged intermediates. ***(06 hrs)***

Outer sphere electron transfer reaction mechanism: elementary steps, precursor and successor complexes. chemical activation-Frank-Condon consideration. ***(05 hrs)***

Elementary idea to Marcus equation, Marcus cross equation. orbital symmetry considerations. differentiation of inner sphere and outer sphere electron transfer reactions. electron transfer reaction in metalloproteins (elementary idea). ***(04 hrs)***

Unit-IV Organo-Metallic Compounds (16 Contact hours)

C—C vs M—C bond. Nomenclature and classification of organometallic compounds. Effective atomic number rule and its applicability. ***(03 hrs)***

Stability of Organometallic Compounds towards heat (decomposition pathways) oxidation and hydrolysis. Properties, structure, bonding and applications of Alkyls and aryls of Li, B, Al and Sn. Structure and bonding in Zeise's Salt. DCDM model of bonding in Pi Organometallics. ***(07 hrs)***

Homogenous Catalysis: Designing of a homogenous Transition Metal catalysts. Tolman Catalytic loop. Mechanistic aspects: Oxidative addition, Insertion reactions. Catalytic efficiency: TOF, TON and *e.e*. Selected homogeneous Catalytic processes: Monsanto Acetic acid and Hydrogenation reaction. ***(06 hrs)***

Books Recommended:

1. Advanced Inorganic Chemistry, 6th ed. /5th ed. F.A. Cotton , G. Wilkinson (Wiley 1999/1988)
2. Inorganic Chemistry, 4th ed. J. E. Huheey, E. A. Keiter..... (Harper Collins, 1993)
3. Chemistry of the Elements 2nd ed. - N. N. Greenwood, A. Earnshaw (Butterworth, 1997)
4. Mechanisms of Inorganic Reactions - D. Katakis, G. Gordon (Wiley, 1987)
5. Reaction Mechanism of Inorganic and Organometallic systems, 2nd ed.- R. B. Jordan (Oxford, 1998)
6. Mechanisms of Inorganic Reactions, 2nd ed. - F. Basolo, R.G. Pearson (Wiley, 1967)
7. Inorganic Chemistry- K. F. Purcell, 1C. Kotz (Saunders, 1977).
8. Principles of Organometallic Chemistry, P. Powell, Chapman and Hall; 2nd ed. 1988
9. Basic Organometallic Chemistry, concepts, synthesis and applications, B.D Gupta, A. j Elias, Universities Press; 2nd edition (1 January 2013)
10. Organometallics and Catalysis: An Introduction, OUP Oxford; UK ed. edition 2014.

Course No: CH24202CR
Title: Organic Chemistry (04 Credits)

Max. Marks: 100 **Duration: 64 Contact hours**

Continuous Assessment: 20 marks **End Term Exam: 80 Marks**

Course outcomes:

- To understand the nature of C=O bonds and C=C multiple bonds in organic compounds.
- Recognize the rearrangements around carbons, importance and understand different aspects of stereochemistry.
- Comprehend the photochemical reactions, photo sensitizers and electronic excitations
- Perceive the concepts of pericyclic reactions, Orbital symmetry and detailed concerted mechanisms

Unit-I Reaction Mechanism-III (16 Contact hours)

Addition to carbon-oxygen double bond:

Nucleophilic additions, stereochemical aspects through various models (Cram, Cram chelation and Felkin-Anh models). ***(2 hrs)***

Enolate Chemistry (Lithium enolates and enamines). Mechanism and stereochemical aspects of condensation reactions (Aldol, Claisen, Knovengeal, Benzoin, Stobbes), Micheal addition, Robinson annulations. ***(5 hrs)***

Addition of Phosphorus (Witting reaction) and sulfur ylides. Wittig-Horner & Corey-Fuchs reaction. ***(2 hrs)***

Addition to carbon-carbon multiple bonds:

Stereochemical implications of addition reactions involving electrophiles and nucleophiles. Hydroboration and Epoxidation, regioselectivity of epoxide ring opening. ***(4 hrs)***

Hydrogenation of double/triple bonds and aromatic rings. Hydration of alkynes. Addition to dienes, 1,2- vs 1,4-additions. ***(3 hrs)***

Unit-II Molecular Rearrangements (16 Contact hours)

General mechanistic treatment of nucleophilic, electrophilic and free radical rearrangements. Nature of migration and migratory aptitude, and memory effect. ***(5 hrs)***

Detailed mechanistic and stereochemical implications involved in the following rearrangements. Wagner-Meerwein, Pinacol, Semipinacol, Demyanov, Benzil-Benzilic acid, Favorskii, Arndt-Eistert, Neber, Hofmann, Curtius, Lossen, Schmidt, Beckmann, Baeyer-Villiger, Pyne and Dienone - phenol rearrangements. ***(11 hrs)***

Unit-III Photochemistry (16 Contact hours)

Interaction of electromagnetic radiation with matter. Types of excitations. Singlet and triplet states. Fate of excited molecule. ***(2 hrs)***

Photochemical reactions of alkenes: Photoinduced geometrical isomerization, photochemical reactions of 1,3; 1,4 and 1,5 dienes. ***(3 hrs)***

Photochemical reactions of Carbonyl compounds: Acyclic and cyclic saturated carbonyl compounds (Norrish type I and Norrish type II reactions), α, β- and β,γ- unsaturated ketones, cyclohexenones and cyclohexadienones. Intermolecular cycloaddition reactions (Paterno- Buchi reaction). ***(5 hrs)***

Photochemical reactions of benzene and its derivatives: Photoisomerizations of benzene and its alkyl derivatives. Nucleophilic photosubstitutions in aromatic compounds. Photo-Fries rearrangements of aryl esters. Barton and Hoffmann-Loefter-Freytag reactions. ***(6 hrs)***

Unit-IV Pericyclic Reactions (16 Contact hours)

Molecular orbital symmetry, Frontier orbitals of ethene, 1,3- butadiene, 1,3,5-hexatriene and allylic systems. HOMO, LUMO concept, FMO approach. Classification of Pericyclic reactions. Woodward Hofmann rules for conservation of symmetry. ***(4 hrs)***

Cycloadditions: Thermal and Photochemical 2+2 and 4+2 cycloadditions. Regioselectivity in 2 + 2 and Diels Alder reactions. Alder-Ene reaction and 1,3 dipolar cycloadditions. Suprafacial and Antrafacial cycloadditions. ***(5 hrs)***

Electrocyclic Reactions: Thermal and Photo-induced Electrocyclic reactions of 4n and 4n + 2 systems and their stereochemistry. Conrotatory and disrotatory motions. ***(4 hrs)***

Sigmatropic rearrangements: Introduction, classification and mechanistic details of [1,3], [1,5], [1,7], [2,3] and [3,3]sigmatropic shifts. Cope and Claisen rearrangements. Suprafacial and Antrafacial shifts of hydrogen atom. ***(3 hrs)***

Books Recommended

1. March's Advanced Organic Chemistry Reactions, Mechanism and Structure, 6thEd., Smith, M.B. (Wiley-2014)
2. Organic Chemistry 8th Ed. - F. A. Carey and Robert M. Giuliano (McGraw Hill-2012).
3. Reaction Mechanism in Organic Chemistry RevisedEd., S.M. Mukherjee and S.P. Singh. (Macmillan- 2017).
4. Organic Chemistry - 2nd Ed., J. Hornback. (Brooks/Cole- 2006).
5. Organic Chemistry, 5th Ed., John McMurry. (Brooks/Cole-2000).
6. Advanced Organic Chemistry, 5th Ed., F.A Carey & R.J Sundberg (Springer-2007).
7. Organic Chemistry, 2nd Ed., Jonathan Clayden (OUP-2016).
8. Organic Chemistry, 11th Ed., Solomons, T.W.G., (Wiley-2015).
9. Organic chemistry, Morrison, Boyd and Bhattacharya. 7th Ed. Pearson-2013.
10. Introductory Photochemistry, A. Cox and T. Kemp (McGraw Hall-1971).
11. Organic Photochemistry, 2nd Ed., J. Coxon, and B. Halton (2nd Ed. Cambridge University press-1987).

Course No: CH24203CR
Title: Physical Chemistry (04 Credits)

Max. Marks: 100 **Duration: 64 Contact hours**
Continuous Assessment: 20 marks **End Term Exam: 80 Marks**

Course outcomes: After studying this course, the students shall:

- get familiar with the orbital and spin angular momenta of electrons and learn to evaluate the permissible energy pattern of atoms through coupling schemes.
- learn variation and perturbation theories for evaluating the approximate properties of atoms/molecules and their applications in bonding theories.
- be able to appreciate the special physicochemical aspects and implications of solid-liquid, liquid-liquid and liquid-air interfaces.
- learn the basic concepts of statistical thermodynamics like thermodynamic probability, distribution functions and distribution laws
- be able to make use of statistical thermodynamic concepts for the estimation of thermodynamic parameters of systems like ideal gases, ideal and non-ideal solutions and monoatomic solids
- learn about the concept of nuclear spin and its implications over the thermodynamic and spectroscopic properties of simple systems.

Unit-I Quantum Chemistry-II (16 Contact hours)

General theory of angular momentum. Eigen functions and Eigen values of angular momentum operators. Ladder operators. ***(3 hrs)***

Spin angular momentum, Atomic term symbols, term separation of p^n and d^n configurations, spin-orbit coupling, Zeeman splitting. ***(3 hrs)***

Approximation methods: The Variation theorem, linear variation principle, application to hydrogen atom and helium atom. ***(3 hrs)***

Perturbation theory: first order (non-degenerate & degenerate). Application of perturbation method to helium atom and anharmonic oscillator. ***(3 hrs)***

Chemical Bonding: LCAO-MO approximation, H_2^+ molecular ion, brief introduction to H_2. Valence bond treatment of hydrogen molecule, comparison of MO and VB methods in the light of hydrogen molecule. ***(4 hrs)***

Unit-II Surface Chemistry (16 Contact hours)

Liquid Surface: Surface tension, pressure difference across curved surfaces (Laplace equation), vapor pressure of droplets (Kelvin equation), Capillary condensation. ***(5 hrs)***

Thermodynamics of Interfaces: Relation between surface excess, surface tension and thermodynamic parameters, Gibbs adsorption isotherm. ***(3 hrs)***

Solid liquid interface: Contact angle, Young's equation, wetting and contact angle. ***(3 hrs)***

Solid surfaces: Adsorption at solid surfaces: types, adsorption models: Langmuir adsorption isotherm, BET adsorption isotherm and its use in estimation of surface area. Adsorption on porous solids. ***(5 hrs)***

Unit-III Statistical Thermodynamics-I (16 Contact hours)

Probability theory: Probability, Fundamental counting principle, Permutations, Configurations, Concept of distribution, thermodynamic probability and most probable distribution. Sterling approximation. ***(6 hrs)***

Distribution Laws: Derivation of Boltzmann, Bose-Einstein and Fermi- Dirac laws distribution laws and their comparison. ***(4 hrs)***

Partition function & its significance. Translational, rotational, vibrational and electronic partition functions. Relation between partition function and thermodynamic functions. ***(4 hrs)***

Ensembles: Concept of ensembles, ensemble average and postulate of equal-a-priori probability. Canonical, grand-canonical and micro-canonical ensembles (Concept only). ***(2 hrs)***

Unit-IV Statistical Thermodynamics-II (16 Contact hours)

Application to Chemical Systems: Calculation of thermodynamic properties in terms of partition functions for ideal monoatomic & diatomic gases. Equilibrium constant in terms of partition functions with application to isomerization and atomization reactions. ***(6 hrs)***

Applications of distribution laws: Distribution of molecular velocities in ideal gases, Black body radiations, electron gas in metals. ***(3 hrs)***

Nuclear spin statistics: symmetry and nuclear spin, ortho and para nuclear spin states, ortho and para hydrogen/deuterium, CO. ***(3 hrs)***

Statistical mechanics of solids: Einstein and Debye models (Partition function, average energy and heat capacity), and their limitations. ***(4 hrs)***

Books Recommended:

1. Atkins' Physical Chemistry, Peter William Atkins, Julio De Paula, & James Keeler, 12th Edition, Oxford University Press, 2023.
2. Physical Chemistry- A Molecular Approach - D. A. McQuarie & J. D. Simon, University Science Books, 1997.
3. Introduction to Quantum chemistry - A. K. Chandra, TataMcGraw Hill, 1997.
4. Quantum Chemistry - Ira. N. Levine, 7th Edition, Pearson, 2014.
5. Quantum Chemistry, R. K. Prasad, 2nd Edition, New Age Publishers, 2001.
6. Physics and Chemistry of Interfaces, H-J, Butt, K. Graf and M. Kappl, 2nd Edition, Wiley-VCH Verlag Gmbh and Co. KGaA, 2006.
7. Physical Chemistry of Surfaces, A. W. Adamson and A. P. Gast, 6th Edition, John Wiley and Sons, Inc. 1997.
8. Statistical Thermodynamics, M. C. Gupta, New Age International, 1993.
9. Statistical Mechanics, Agarwal, Eisner, Wiley, 1991.
10. Statistical Thermodynamics-Fundamentals and Applications, N.M. Laurendeau, Cambridge University Press, 2005.

Course No: CH24204CR
Title: Green Chemistry (02 Credits)

Max. Marks: 50 **Duration: 32 Contact hours**
Continuous Assessment: 10 marks **End Term Exam: 40 Marks**

Course outcomes: On completion of the course, the student should be able to:

- To understand the fundamentals of green chemistry. Green Solvents, Catalysts and Green Reactions
- Understand the principles of Green Chemistry.
- Understand the basics of organic reactions with special context to green Chemistry.
- Understand need of green chemistry

Unit-I Green Chemistry-Theory (16 Contact hours)

Introduction: Need for Green Chemistry and the role of chemists. ***(2 hrs)***
Principles of Green Chemistry and its tools: selection of starting materials, catalysts, alternative solvents, appropriate reagents, percentage atom utilization. microwaves, sonication and visible light. ***(6 hrs)***
Green Solvents and Reaction conditions: Supercritical fluids, Aqueous reaction conditions, Immobilized Solvents and irradiative reaction conditions. Examples of green materials, and reagents. ***(8 hrs)***

Unit-II Green Reactions (16 Contact hours)

Reactions carried under green conditions, acyloin condensation with mechanism, acyloin condensation using co-enzyme- Thiamine. ***(3 hrs)***
Aldol condensation with mechanism using green reagents -ionic liquids, super critical water and solid phase. ***(3 hrs)***
Baeyer-Villiger oxidation in an aqueous medium, solid phase and enzyme catalyzed. ***(2 hrs)***
Baylis-Hillman reaction using microwave technique and in polyethylene glycol. ***(3 hrs)***
Benzoin condensation under green conditions. Dakin reaction with mechanism using ultrasonic irradiation. ***(3 hrs)***
Darzen reaction with mechanism in presence of phase transfer catalyst (PTC). ***(2 hrs)***

Books recommended

1. Green Chemistry- Environment Friendly Alternatives; Rashmi Sanghi& M. M Srivastava; Narosa; 2007.
2. Green Chemistry- An Introductory Text; IIndEdn.; Mike Lancaster; RSC; **2010.**
3. Green Chemistry- Theory and Practice; P. T. Anastas and J. C. Warner; oxford; **2000**.
4. Green Chemistry –Environmentally Benign Reactions; V.K.Ahluwalia, 2nd Edition, **2012**
5. Green Chemistry, Rashmi Sanghi and M M Srivastava; **2003** 1st Edition
6. Research papers **2012** to **2018**, (Journals recommended, Green Chemistry, Asia's Sustainable Chemistry, JOC, OL, Tetrahedron Letters, Catalysis Communications, JSCS, RSC Advances, NJC, Chemistry select, Molecular catalysis A chemical, Catalysis Letters).

Course No: CH24205DCE
Title: Laboratory Course in Chemistry-II (4 Credits)

Max. Marks: 100 **Duration: 128 Contact hours**
Continuous Assessment: 20 marks **End Term Exam: 80 Marks**

Course outcomes: After performing this lab course, the students will be able

- To know about Multi stage organic Preparations, purification and identification of different functional moiety in the compound.
- To know about Natural product Isolation/extraction.
- To know about Estimation of unknown quantity in a given sample.
- To know about Chromatography.

1. **Separation, Purification and identification of Organic compounds from two component mixture.**

2. **Qualitative Analyses of Organic Compounds**
   (a) Physical & Chemical Properties: Physical state, colour, odour, solubility behaviour and melting / boiling points. Flame test
   (b) Detection of elements: Nitrogen, Sulphur and Halogens
   (c) Detection of Functional Groups: Detection of Carbohydrates, Unsaturation, Carboxylic acids, Carbonyl compounds, Phenols, Alcohols, Halides, Amines, Amides, Imides, Ureas, Thio ureas, Nitrocompounds and Hydrocarbons

3. **Organic Preparations (two and three step syntheses)**
   Condensation reactions (Aldol), Chemoselective synthesis (Aspirin), Rearrangement (Beckmann), Diels alder reaction , Acetylation reaction (Acetanilide synthesis), Synthesis of Sulphanilamide (Sulpha drug), Oxidation of Cyclohexanol by chromic acid to get adipic acid.
   Crystallization, MPt and Characterization of Synthesized Compounds by IR spectroscopy.

4. **Isolation/Extraction of following natural products.**
   Citric acid from Lemon, Lycopene from Tomato, caffeine from Tea.
   (Characterization by IR/UV spectroscopy)

5. **Quantitative Estimation of Glucose and Glycine: Using Volumetric Analyses**

6. **Separation & identification of given amino acid mixture using paper Chromatography.**

Books Recommended:

1. Experiments and Techniques in Organic Chemistry - D. Pasto, C. Johnson and M. Miller (Prentice-hall, 1992.)
2. Microscale and Macroscale Organic Experiments- K.L. Williamson (D.C. Heath and Co., 1989).
3. Advanced Practical Organic Chemistry, 2nd ed. - N.K. Vishnoi (Vikas, 1999).
4. Vogel's Textbook of Practical Organic Chemistry, 5th ed.- A.R. Tatchell (ELBS, • 1996)
5. Comprehensive Practical Organic Chemistry, V. K. Ahluwalia and Renu Aggarwal, (University Press-2000)

Course No: CH24206 DCE
Title: Bio-inorganic chemistry (02 Credits)

Max. Marks: 50 **Duration: 32 Contact hours**
Continuous Assessment: 10 marks **End Term Exam: 40 Marks**

Course outcomes: The students are expected to:

- learn the importance of inorganic elements in biological systems.
- understand the chemistry and biology of specific bioinorganic systems and model metal complexes.
- appreciate and recognize how the fundamental principles of inorganic chemistry apply to bioinorganic systems.
- understand the application of specialized methods used to study bioinorganic molecules.
- understand inorganic chemistry at the biological interface.
- understand structure and mechanistic importance of metal ions in functioning of selective biological molecules.

Unit-I Bioinorganic systems (16 Contact hours)

Alkali and alkaline earth metals in biology; (Na^+-K^+ pump, ionophores). Structure and coordinating sites in biologically important ligands. Metal ion transport: (uniport, symport and antiport), siderophores and metallothionein. ***(03 hrs)***

Iron Storage, Transport and Oxygen carriers: Ferritin and Transferrin: Structure, Metal binding sites; incorporation and release of iron. Hemoglobin and Myoglobin: Structure, oxygen saturation curves; mechanism of oxygen transport and storage. Bohr Effect and cooperativity in hemoglobin. Dioxygen binding to hemerythrin and hemocyanin. Synthetic oxygen carrier model compounds. ***(08 hrs)***

Metalloenzymes: Structure and function of carbonic anhydrase, carboxy peptidase, catalase, superoxide dismutase. ***(05 hrs)***

Unit-II Biological Electron transport and chelation therapy (16 Contact hours)

Electron Carriers: Structure and biological role of Rubredoxin & Ferredoxin, Cytochromes as electron transfer proteins. Nitrogenase enzyme and its role in biological nitrogen fixation. ***(05 hrs)***

Metal homeostasis and related diseases. Chelation therapy: Therapeutic aspects of chelating drugs:-conditional stability constant, stereochemistry, lipophilicity. HSAB theory and plasma mobilizing index(PMI). Types of chelation therapy: single, double, synergistic and mixed ligand chelation therapy. Therapeutic index of different chelating drugs in metal ion detoxification. Radio protective chelating drugs. Limitations and hazards of chelation therapy. ***(08 hrs)***

Drug Biotarget interactions: Biophysical and spectroscopic methods of drug binding to serum albumins, DNA and enzymes. ***(03 hrs)***

Books Recommended:

1. Principles of Bioinorganic Chemistry; S. J. Lippard and J. M. Berg; University Science Books;1994.
2. Bioinorganic Chemistry, D. Rehder, Oxford University Press; 2014.
3. The Inorganic Chemistry of Biological Processes; 2nd edn.; M. N. Hughes; John Wiley;1973.
4. Inorganic Chemistry in Biology, P. C. Wilkins, G. Wilkins, OUP Oxford, , 1997
5. Physical methods in bioinorganic chemistry: spectroscopy and magnetism; L.Que, University Science Books,U.S.; Reprint edition 2010.
6. Bioinorganic Chemistry- A Short Course; R. M. Roat, Malone; Wiley Interscience;2003.
7. Inorganic Chemistry Principles of Structure and Reactivity 4th, 5th edn:, J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, Pearson Education; 2022
8. Techniques and topics in bioinorganic chemistry, C.A. Mcauliffe, John wiley,1975.
9. Bioinorganic chemistry: Inorganic elements in the chemistry of life, W.Kaim, B. Schwederski, A. Klein, Wiley, 2013.
10. Concepts and Models in Bioinorganic Chemistry, H, B. Kraatz, N. M. Nolte, Wiley-VCH Verlag GmbH; 1st edn, 2006

Course No: CH24207DCE
Title: NMR and ESR Spectroscopy (02 Credits)

Max. Marks: 50 **Duration: 32 Contact hours**
Continuous Assessment: 10 marks **End Term Exam: 40 Marks**

Course Outcomes: After studying this course, the students will

- know how nuclear spins are affected by a magnetic field and how to interpret peaks in an NMR spectrum of a compound.
- utilize the coupling constants for determining compound structure.
- learn the principle and instrumentation of electron spin resonance spectroscopy and apply the knowledge in characterizing the molecules.

Unit-I: NMR Spectroscopy (16 Contact hours)

Basic principles: Nuclear spin, spin angular momentum, nuclear magnetic moment, precessional (Larmor) frequency, energy levels in a magnetic field, resonance absorption of radio frequency radiation, population of energy levels, Relaxation processes (T1, and T2). ***(04 hrs)***
Shielding and deshielding of magnetic nuclei, Chemical shift and factors affecting chemical shifts: local paramagnetic and diamagnetic shielding, neighboring group anisotropy and ring currents in aromatic systems, Spin- Spin coupling, coupling constants and factors influencing coupling constants. ***(07 hrs)***
Double resonance techniques; spin decoupling, nuclear Overhauser enhancement.
Instrumentation; FT-NMR and its advantages. NMR studies of nuclei other than proton – ^{13}C, ^{19}F and ^{31}P. ***(05 hrs)***

Unit-II ESR Spectroscopy (16 Contact hours)

Basic principles- electron spin, magnetic moment of an electron and its interaction with applied magnetic field. Splitting of spin energy states and absorption of microwave radiation. ***(6 hrs)***
Hyperfine coupling, Isotropic and anisotropic hyperfine coupling constants, Examples, Fermi contact, Spin polarization effects, Dipolar coupling, Mc Conell equation and calculation of spin densities in inorganic radicals such as $CO_2^{-\bullet}$, $CH_3^{\bullet}$, $BH_3^{-\bullet}$ and $F_2^{-\bullet}$. ***(6 hrs)***
Spin orbit coupling and significance of g tensors. Zero field splitting and Kramer's degeneracy (fine structure), Advance Applications ***(4 hrs)***

Books Recommended

1. Introduction to Electron Spin Resonance; H. M. Assenheim; Springer, 2014.
2. Introduction to Magnetic Resonance Spectroscopy ESR, NMR, NQR; 2nd edn.; D.N. Sathyanarayana; I K International Publishing House,2013.
3. Understanding NMR Spectroscopy; 2nd edn.; J. Keeler; Wiley-Blackwell;2010.

4. Introduction to Spectroscopy; 4th edn.; D. L. Pavia, G. M. Lampman, G. S. Kriz, J. Vyvyan; Cengage Learning, 2008.
5. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry; R. V. Parish;Ellis Horwood; 1990.
6. Nuclear Magnetic Resonance; P. J. Hore; Oxford;1995.
7. Nuclear Magnetic Resonance Spectroscopy; A physicochemical View; R. K. Harris;Pitman Publishing1983,
8. Principles of Instrumental Analysis; 4th edn.; D. A. Skoog, J. J. Leary; Saunders;1992.
9. Physical Methods for Chemists; 2nd edn.; R. S. Drago; Saunders;1992.
10. Basic Principles of Spectroscopy; R. Chang; McGraw Hill;1971.
11. Introduction to Magnetic Resonance; A Carrington, A. D. McLachlan; Harper & Row;1967.
12. NMR and Chemistry; 2nd edn.; J. W. Akitt; Chapman and Hall;1983.

Course No: CH24002GE
Title: Metal Ions in Living Systems (02 Credits)

Max. Marks: 50 **Duration: 32 Contact hours**
Continuous Assessment: 10 marks **End Term Exam: 40 Marks**

Course outcomes: The students are expected to:

- learn the importance of inorganic elements in vital systems.
- understand the chemistry and biology of specific bioinorganic systems and model metal complexes.
- appreciate how nature acquires and places trace elements for use in life processes.
- recognize how the fundamental principles of inorganic chemistry apply to bioinorganic systems.
- understand the application of specialized methods used to study bioinorganic molecules.
- understand metal ion binding to biomolecules and their functions.
- demonstrate an advanced understanding of the key differences in the roles of metal containing systems in biology.

Unit-I Metal-ions in Bio-systems: (16 Contact hours)

Classification of metals according to their action in biological systems. Metal coordination behavior of biomolecules. Concept of essentiality, criteria and classification of essential elements. Metal Homeostasis and related diseases. Structure and Coordinating sites in biologically important ligands: Proteins, Nucleotides and Lipids. ***(8 hrs)***

The transport mechanism: uniport, symport and antiport. Alkali Metals: Role of Sodium and Potassium, mechanism of transport across the cell membrane. Role of Lithium in mental health. Alkaline Earth Metals: Role of Calcium in muscle contraction and blood clotting. Role of Magnesium in chlorophyll. Toxicity of metals: Arsenic, Mercury, Cadmium and Lead. Cyanide Toxicity, Metallothioneins. ***(8 hrs)***

Unit-II Biological Activity of Essential Trace Elements (16 Contact hours)

Iron: Storage and transport through Ferritin and Transferrin. Hemoglobin and Myoglobin: Structure, iron binding sites and role of iron in oxygen transport. ***(4 hrs)***

Copper in Biochemical systems: Electron transfer, oxidation and oxygenation of substrates. Zinc in Biosystems: Lewis acid catalyst, Enzyme activator in vitamin B_{12}. Biochemical basis of essential metal deficient diseases and their therapies (Iron, Zinc, Copper and Manganese). ***(6 hrs)***

Metal complex as drugs: Platinum, Rhodium and Gold complexes. Antibacterial, Antiviral and Antifungal activities of metal complexes with probable mechanism of action. ***(4 hrs)***

Books Recommended:

1. 1. Principles of Bioinorganic Chemistry; S. J. Lippard and J. M. Berg; University Science Books, 1994.
2. Bioinorganic Chemistry- An introduction; Ochiai; Allyn and Bacon, 1977.

3. Bioinorganic Chemistry - Inorganic Elements In The Chemistry Of Life - An Introduction And Guide, John Wiley, 2013.
4. The Inorganic Chemistry of Biological Processes; 2nd edn, M. N. Hughes, John Wiley, 1973.
5. Bioinorganic Chemistry- A Short Course; R. M. Roat, Malone; Wiley Interscience, 2003.
6. Biological Inorganic Chemistry, Structure and Reactivity I. Bertini, University Science Books, 2007.
7. Bioinorganic Chemistry: Concepts and Models, I. Walker, Callisto Reference, 2022.
8. Inorganic Chemistry : Principles of Structure and Reactivity, 5th edn, J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, Pearson Education, 2022.

Course No: CH24002OE
Title: Chemistry of Bio-Molecules (02 Credits)

Max. Marks: 50 **Duration: 32 Contact hours**
Continuous Assessment: 10 marks **End Term Exam: 40 Marks**

Course outcomes: On completion of the course, the students should be able to:

- understand structure, chemistry and importance of biomolecules.
- understands the Aerobic and Anaerobic metabolism.
- understand enzyme and theories of enzymes.
- understand the chemistry involved in DNA & RNA
- know the importance of micronutrients.

Unit-I (16 Contact hours)

Carbohydrates

Carbohydrates: Definition, classifications. Significance of right and left handedness. Production through photosynthesis Composition and functions of: Monosaccharides: Glucose, Fructose and Galactose. Disaccharides: Sucrose, lactose and Maltose. Invert Sugar. Polysaccharides: Starch, glycogen and Cellulose. Aerobic and Anaerobic metabolism. ***(10 hrs)***

Lipids

Steroids: Cholesterol, transport of Cholesterol in blood stream. Cholesterol and heart diseases, Recommended values of HDL and LDL , Steroidal hormones and anabolic steroids ***(6 hrs)***

Unit-II (16 Contact hours)

Proteins and Enzymes: Introduction, Amino Acids: Structural features and classification. Primary, Secondary, Tertiary and Quaternary structures of proteins and their significance. Denaturation and Renaturation of proteins. Urea cycle. Enzymes: Classification. Theories of mechanism of action of Enzymes; Fisher Lock and Key Theory, Koshland's Induced Fit Theory. Mechanism of action of Chymotrypsin and Carboxypeptidase. ***(10 hrs)***

Nucleic Acids, Vitamins and Minerals: Nucleic acids: Structural features of nucleotides, Nucleotides: DNA and RNA. Vitamins: Classes of Vitamins and their functions. Vitamin deficiency diseases. ***(6 hrs)***

Books Recommended

1. Organic Chemistry; 5th edn;. Vol.2,1.L.Finar (Addison Wesley Longman-2000).
2. Biochemistry, Biotechnology and Clinical Chemistry of Enzymes; Trevor Palmer (EWP). Organic Chemistry by I.L.Finar; Vol. II (ELBS Longamnn).
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