# Course No: CH21201CR Title: Inorganic Chemistry (04 Credits)

# Max. Marks: 100 Continuous Assessment: 20 marks

# Duration: 64 Contact hours End Term Exam: 80 Marks

**Course Outcome:** The course focus on learning of inorganic reaction mechanism, which is generally not taught in good detail at the undergraduate level. Besides helping the students to understand structure of intermediates and the influence of different factors on the fate of a reaction, the course develops the temperament of a student for reaction design and control. The courses also provides understanding about the 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.

General reaction mechanism of square planar complexes, KS and KY pathways. Nature of reaction intermediates/ transition states. 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 theories and application in synthesis, Trans influence. Cis-effect. Nature of entering group. Affect of central metal atom.

Molecular rearrangements in 4-coordinate complexes.

# Unit-II Mechanisms of Ligand Substitution Reactions in Octahedral Metal Complexes (16 Contact hours)

Reactivity of metal complexes-Kinetic and thermodynamic stability, Identification inert and labile complexes. Rate laws.

Types of substitution reactions; mechanistic classification of substitution reactions:-Dissociative, Associative, and Interchange mechanism. Empirical criteria to differentiate the mechanism of substitution reaction.

Substitution in octahedral complexes-Replacement of coordinated-Mechanism, Rates of water replacement.

Classification of metal ions based on water exchange rates.

Eigen-Wilkins mechanism. Anation reactions.

Solvolysis/Hydrolysis: Hydrolysis under acidic conditions, Hydrolysis under basic conditions- Conjugate base (CB) mechanism.

Substitution reactions without breaking of metal-ligand bond.

# Unit-III Mechanism of Electron Transfer Reactions in Coordination Complexes

# (16 Contact hours)

(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.

Outer Sphere Electron Transfer Reaction Mechanism: Elementary steps, precursor and successor complexes. Chemical activation-Frank-Condon consideration. 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).

# **Unit-IV Organo-Metallic Compounds:**

Introduction, C—C vs M—C bond. Nomenclature and classification of organometallic compounds. Effective atomic number rule and its applicability. 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. Synthesis, Structure and bonding in Zeise's Salt. DCDM model of bonding in Pi organometallics. Homogenous Catalysis Mechanistic aspects: Oxidative addition, Insertion reactions and water gas shift reaction(WGSR) and C—H activation. Designing of a homogenous Transition Metal catalyst. Tolman Catalytic loop. Catalytic efficiency: TOF, TON and e.e. Selected Industrial Catalytic processes: Hydrogenation ,Hydroformation, Monsanto Acetic

acid and Reppe reaction.

### **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. Electronic Spectra of Transition Metal Complexes D. Sutton (McGraw-Hill, 1968)
- 9. Elements of Magnetochemistry R. L. Dutta, A. Syamal (Affiliated East -West, 1993)

# Course No: CH21202CR **Title: Organic Chemistry (04 Credits)**

# Max. Marks: 100 **Continuous Assessment: 20 marks**

# **Duration: 64 Contact hours End Term Exam: 80 Marks**

**Course Outcome:** On completion of the course, the students should be able 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**

Addition to Carbon-Oxygen double bond: Nucleophilic additions to carbonyls and stereochemical aspects through various models (Cram, Cram chelation and Felkin-Anh models), Review of mechanisms of addition of water, hydrogen cyanide, alcohols, amines, organometallic reagents and hydrides to aldehydes and ketones. Mechanism and stereochemical aspects of Aldol reactions (Controlling aldol reactions, intramolecular Aldol reaction and Cross Aldol condensation), Knoevenagel reaction, Robinson annulation, Claisen and cross Claisen ester condensation. Dickman and Stobbes reactions. Addition of Phosphorus, nitrogen and sulfur ylids. Wittig-Horner reaction.

Addition to carbon-carbon multiple bonds: General mechanism, reactivity, orientation and stereochemical implications of addition reactions involving electrophiles, nucleophiles and free radicals. Hydrogenation of double/triple bonds and aromatic rings. Hydration of alkynes. Hydroboration and Epoxidation, regioselectivity of epoxide opening.

Conjugate additions: Addition to dienes and  $\alpha$ ,  $\beta$ -unsaturated systems. Micheal addition, addition of lithium enolates and enamines. 1,2- vs 1,4-additions.

# **Unit-II Molecular Rearrangements**

General mechanistic treatment of nucleophilic, electrophilic and free radical rearrangements. Nature of migration and migratory aptitude, and memory effect. 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.

# **Unit-III Photochemistry**

Interaction of electromagnetic radiation with matter. Types of excitations. Singlet and triplet states. Fate of excited molecule: Physical (Jablonski diagram) and chemical processes. Sensitization and Quenching.

Photochemical reactions of alkenes (Geometrical isomerization) and 1,3, 1,4 and 1,5 dienes. Photochemistry of Carbonyl compounds: Photochemical reactions of acyclic and cyclic saturated carbonyl compounds (Norrish type I and II reactions),  $\alpha$ ,  $\beta$ - and  $\beta$ ,  $\gamma$ - unsaturated ketones, cyclohexenones and cyclohexadienones. Intermolecular cycloaddition reactions (Paterno- Buchi reaction).

Photoisomerizations of benzenes and its alkyl derivatives. Nucleophilic photosubstitutions in aromatic compounds. Photo-Fries rearrangements of aryl esters and anilides. Barton and Hoffmann-Loefter-Freytag reactions.

# (14 Contact hours)

(20 Contact hours)

### **Unit-IV Pericyclic Reactions**

### (14 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.

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.

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

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.

### **Books Recommended**

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

# **Course No: CH21203CR Title: Physical Chemistry (04 Credits)**

# Max. Marks: 100 Continuous Assessment: 20 marks

# Duration: 64 Contact hours End Term Exam: 80 Marks

- **Course outcome:** After learning the contents of 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.
- learn to derive some important equations of thermodynamics and understand the implications of these equations.
- ➤ be able to make use of thermodynamic relations for the thermochemical estimations
- ➢ be able to sketch and read the phase diagrams of three component systems
- 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

*General theory of angular momentum.* Eigen functions and Eigen values of angular momentum operators. Ladder operators. Spin angular momentum, antisymmetry and Pauli's principle. Atomic term symbols, term separation of  $p^n$  and  $d^n$  configurations, spin-orbit coupling, Zeeman splitting.

*Approximation methods:* The Variation theorem, linear variation principle, application tohydrogen atom and helium atom. Perturbation theory: first order (non-degenerate & degenerate). Application of perturbation method to helium atom and anharmonic oscillator. Chemical Bonding: LCAO-MO approximation,  $H_2^+$  molecular ion, brief introduction to  $H_2$ . Molecular term symbols. Valence bond treatment of hydrogen molecule, comparison of MO and VB methods in the light of hydrogen molecule.

# Unit-II Equilibrium Thermodynamics

Maxwell Relations and thermodynamic equations of state.

*Thermodynamics of multicomponent systems:* Partial Molar properties, Partial molar free energy: concept Chemical Potential, Chemical potential variation with Temperature and Pressure, Determination of chemical potential, Applications of chemical potential (Henry's law, Raoult's law and Nernst distribution law), Chemical potential and Gibbs-Duhem equation, Gibbs-Duhem-Margules equation and its application (Konovalov's First and second laws).

*Phase Equilibria:* Phase equilibria of three component systems: CHCl<sub>3</sub>-CH<sub>3</sub>COOH-H<sub>2</sub>O, NH<sub>4</sub>Cl- (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>-H<sub>2</sub>O and Pb-Bi-Sn systems. First and second order phase transitions.

# Unit-III Statistical Thermodynamics-I

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

*Distribution Laws:* Derivation of Boltzmann distribution law, Bose-Einstein and Fermi-Dirac laws and their comparison with Boltzmann distribution law.

### (16 Contact hours)

# (16 Contact hours)

Partition function & its significance. Translational, rotational, vibrational and electronic partition functions. Relation between partition function and thermodynamic functions.

*Ensembles:* Concept of ensembles, ensemble average and postulate of equal-a-priori probability. Canonical, grand-canonical and micro-canonical ensembles. Ensemble partition functions and related thermodynamic functions. Ideal gas in canonical and Grand canonical ensemble.

#### **Unit-IV Statistical Thermodynamics-II**

### (16 Contact hours)

*Application to Chemical Systems:* Calculation of thermodynamic properties in terms of partition functions, application to ideal monoatomic & diatomic gases. Equilibrium constant in terms of partition functions with application to isomerization and atomization reactions. *Nuclear spin statistics:* symmetry and nuclear spin, Ortho and Para nuclear spin states, Ortho and Para Hydrogen and Deuterium, CO.

Statistical thermodynamics of solutions: Lattice model, regular solution theory,

statisticalmechanics of polymer solution, Flory-Huggins theory.

*Statistical mechanics of solids:* Einstein and Debye models (Partition function, Average energy and heat capacity), limitations of the models.

### **Books Recommended:**

- 1. Physical Chemistry -P. W. Atkins, 9th Edition, ELBS, Oxford, 2009.
- 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, 2009.
- 5. Quantum Chemistry, R. K. Prasad, 2nd Edition, New Age Publishers, 2001.
- 6. Modern Thermodynamics: From Heat engines to dissipative structures-DilipKondepudi, Ilya Prigogine. John Wiley and sons, reprinted, 2007.
- 7. Thermodynamics: Classical, Statistical and irreversible. Rajaram and Kuriocose, Dorling Kindersley Pvt Ltd, 2013.
- 8. A text book of Physical Chemistry, Thermodynamics and Chemical equilibrium; K.L.Kapoor, MacGraw Hill Education, vol. 2, Ed. 6th, 2019.
- 9. Statistical Thermodynamics, M.C.Gupta, New Age International, 1993.
- 10. Statistical Mechanics, Agarwal, Eisner, Wiley, 1991.
- 11. Statistical Thermodynamics-Fundamentals and Applications, N.M. Laurendeau, Cambridge University Press, 2005.

# **Course No: CH21204CR Title: Green Chemistry (02 Credits)**

### Max. Marks: 50 **Continuous Assessment: 10 marks**

# **Duration: 32 Contact hours** End Term Exam: 40 Marks

**Course Outcome:** 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. Principles of GreenChemistry. Tools of Green Chemistry: Selection of starting materials, Catalysts, Alternative Solvents, Appropriate reagents, Percentage atom utilization. Microwaves, Sonication and Visible light. Green Solvents and Reaction conditions: Supercritical fluids, reaction conditions. Immobilized Solvents and irradiative Aqueous reaction conditions. Examples of Greenmaterials, reagents and some specific reactions.

# **Unit-II Green Reactions**

Reactions carried under green conditions, Acyloin Condensation with Mechanism, Acyloin Condensation using Co-enzyme- Thiamine. Aldol condensation with Mechanism using green reagents -Ionic liquids, Super Critical Water and solid phase. Baeyer-Villiger Oxidation in an aqueous medium, solid phase and enzyme catalyzed. Baylis-Hillman Reaction using microwave technique, Supercritical carbon dioxide and polyethylene glycol. Benzoin Condensation under green conditions. Dakin Reaction with mechanism using Ultrasonic Irradiation. Darzen Reaction with mechanism in presence of Phase Transfer Catalyst (PTC). synthesis of heterocyclic Green reactions involving compounds (Benzofuran, Imidazopyridine, Benzothiazole -2 (3H)-one, Isocoumarins and Monobenzoylation reaction.

# **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: CH21205DCE Title: Laboratory Course in Chemistry II (4 Credits)** 

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

- > To know about Multi stage Inorganic Preparations.
- To know about Potentiometric Titrations.
- > To know about pH-metric Titrations.

**Continuous Assessment: 20 marks** 

Max. Marks: 100

> To know about conductometric Titrations

### SECTION A-INORGANIC CHEMISTRY

#### A: -Multi stage Inorganic Preparations:

Preparation of tetraamminecarbonatocobalt (III) nitrate and its conversion to pentaamminecholorocobalt(III)chloride.

• Preparation of Trans-dicholorobis(ethylenediamine) cobalt (III) chloride and its conversion to cis-isomer.

• Preparation of tris(ethylenediamine) nickel (II) chloride dehydrate and analysis of stepwise complexation process

• Preparation of Potassiumtrisoxalatoferrate(III)trihydrate and its component analysis.

• Preparation of Pentaamminecholorocobalt(III) chloride and study of Linkage isomers by its conversion topentaamminenitritocobalt(III) chloride and to nitro isomer followed by IR Characterization.

### **B: - PotentiometricTitrations:**

• Fun with Nernst equation: Standardization of an Iron (ii) solution with a standard dichromate solution and calculation of formal and transition potential values.

• Complexation effect on redox potential of iron redox couple: Simultaneous potentiometric estimation of iron binary and ternary complex mixtures.

• Argentometry :Estimation of Iodide with Standard AgNO<sub>3</sub>overPt&Calomel assembly using I -  $\setminus$  I<sub>2</sub> redox coupleinvolving pseudo indicator action.

. Complexometric titration for determination of Ferro cyanide with standard Zinc (II) solution in order to establish the composition of the complex  $K_2Zn_3[Fe(CN)_6]_2$ 

### **C. pH-metricTitrations:**

• Quantitative analysis of Chromate Dichromate mixture by pH Titration.

• Study of pH influence on a pH dependent redox reaction.

### **D: - ConductometricTitrations:**

(Any 1 Experiment) • Conductometric investigation of Silver(I) ethylenediaminecomplexationreaction.

• Conductometric analysis of a strong binary acid mixture (HNO<sub>3</sub> and H<sub>2</sub>SO<sub>4</sub>)

### SECTION B-ORGANIC CHEMISTRY

Separation, Purification and identification of Organic compounds from a three-1. component mixture

#### 2. **Organic Preparations**

- Bromination of Acetone using NBS & PTS (a)
- Amidation Reaction (b)
- (c) **Acetylation Reactions**
- (d) Haloform reaction: Preparation of Iodoform.

### (Any 1 Experiment)

# (Any 03 Experiments)

# (Any 03 Experiments)

# **Duration: 128 Contact hours** End Term Exam: 80 Marks

- (e) Oxidation of Cyclohexanol by chromic acid to get adipic acid.
- (f) Crystallization, m.p. determination and Characterization of Synthesized Compounds.

### SECTION C-PHYSICAL CHEMISTRY

# A. <u>Conductometry</u>

- 1. Determination of equivalent conductance, degree of dissociation and the dissociation of a weak acid.
- 2. Determination of the composition of a mixture of HCl and CH<sub>3</sub>COOH by titration with standard NaOH.
- 3. Precipitation titration of  $BaCl_2$  and  $K_2SO_4/(NH_4)_2SO_4$
- 4. Estimation of the concentrations of H<sub>2</sub>SO<sub>4</sub>, CH<sub>3</sub>COOH and CuSO<sub>4</sub> in a mixture.

# B. Phase Equilibria

- 1. Investigate the mutual solubility of phenol and water at various temperatures and hence determine the critical solution temperature of phenol-water system.
- 2. Study the effect of addition of NaCl/Succinic acid on the critical solution temperature of Phenol-Water System.
- 3. Investigate the solubility of three component systems and hence draw a tie line on binodal curve.

### 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. Comprehensicve Practical Organic Chemistry, V. K. Ahluwalia and Renu Aggarwal, (University Press-2000)
- 6. Practical Physical Chemistry, Findley, Kitchener, Longman, 1977.
- 7. Advanced Practical Physical Chemistry, Yadav, Goel Pub, 1994.
- 8. Experiments in Physical Chemistry, 5th ed., Schoemakeret al., MGH, 1989.

# Course No: CH21206DCE Title: NMR and ESR Spectroscopy (02 Credits)

# Max. Marks: 50 Continuous Assessment: 10 marks

# **Duration: 32 Contact hours End Term Exam: 40 Marks**

Course Outcome: After studying this course, the students will be able to

- 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

Basic principles, Nuclear spin, spin angular momentum, quantization of 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, T2). Shielding and deshielding of magnetic nuclei. Chemical shift, its measurement and factors influencing chemical shifts; local paramagnetic and diamagnetic shielding, neighboring group anisotropy and ring currents in aromatic systems Spin- Spin coupling, coupling constants.Examples.

Vicinal coupling and electron correlation. Chemical equivalence and magnetic equivalence. Fermi contact and Dirac Vector Model. Effect of Chemical exchange on spectra. 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  ${}^{31}P$ .

# **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. 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  $^{\bullet}$ , BH  $^{-\bullet}$  and F  $^{-\bullet}$ .

Spin orbit coupling and significance of g tensors. Zero field splitting and Kramer's degeneracy (fine structure), Advance Applications

# Books Recommended

- 1. Introduction to Electron Spin Resonance; H. M. Assenheim; Springer, 2014.
- 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.
- 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.
- 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: CH21207DCE Title: Solid State Chemistry (02 Credits)**

Max. Marks:	50	
<b>Continuous</b> A	Assessment:	10 marks

# Duration: 32 Contact hours End Term Exam: 40 Marks

Course outcome: After learning the contents of this course, the students shall:

- get familiar with X-ray diffraction technique and its use in determining the internal structure of the solid state alongwith the electron density maps.
- learn about the types of defects and their importance in explaining the properties of solids.
- understand the development of theories of solid state starting from free electron approximation to the finite variable potential field approximation of the electrons for classifying the solids as insulators, conductors and semiconductors.
- > get familiarized to the semiconducting, superconducting, magnetic and dielectric properties of solids along with their day-to-day applications.

# **Unit-I Structure and Theories of Solids**

# (16 Contact hours)

*Structure of solids:*Lattice Planes and Miller indices; Bragg equation, Debye-Scherrer method of X-ray structural analysis of crystals, identification of cubic unit cells from systematic absences in diffraction pattern. Structure factor and its relation to intensity and electron density.

*Crystal defects and their types.* Point defects: Schottky and Frenkel defects, Thermodynamics of Schottky and Frenkel defect formation, Colourcentres, Dislocations and their types.

# Theories of solids:

Free electron theory of metals: The Drude and Lorentz Model, Sommerfield Model; Fermi-Dirac distribution function, Density of state and electronic heat capacity.

*Electron Energy Bands:* Energy bands in general periodic potential-Kronig-Penney model. Qualitative band schemes for insulators, semiconductors and metals.

# Unit-II Electric and magnetic properties of Solids

### (16 Contact hours)

*Semiconductors:* Intrinsic & extrinsic semiconductor (n-type & p-type), temperature dependence of charge carriers, p-n junction- devices based on p-n junction (tunnel diode, injection laser).

*Super conductors:* Characteristic properties- Zero resistance, Meissner effect, Heat capacity, Thermal conductivity, absorption of em radiations and Josephson effect. BCS theory of superconductivity, applications of superconductors.

*Dielectric Properties of Solids:* Dielectric constant, Polarization and Polarizability, Piezoelectricity, pyroelectricity and ferroelectricity, ferroelectric materials and their applications.

*Magnetic properties of solids:* origin of magnetism in solids, Diamagnetism, paramagnetism (Langevin's and quantum mechanical formulations), ferromagnetism (Wiess theory), antiferromagnetism and ferrimagnetism. Temperature dependence of magnetization.

### **Books Recommended**

- 1. Physical Chemistry; P. W. Atkins; Julio De Paula, Ed. 10th, Oxford University Press;2014.
- 2. Physical Chemistry- A Molecular Approach D. A. McQuarie& J. D. Simon, University Science Books, 1997.
- 3. Introduction to Solids, Azaroff, Tata McGraw, 1993.
- 4. SolidState Chemistry and its Applications, West, Wiley, 2014.
- 5. The Physical Chemistry of Solids, Borg, Biens, Academic press, 1992.
- 6. Solid State Reactions, Schmalzried, Academic press, 1995.
- 7. Solid State Physics, N.W.Ashcroft and N.D.Mermin, Saunders college, 2001.
- 8. Elements of Solid state Physics, J.P. Srivastava, Prentice Hall of India, 2003

# Course No: CH21002GE Title: Metal Ions in Living Systems (02 Credits)

### Max. Marks: 50 Continuous Assessment: 10 marks

# Duration: 32 Contact hours End Term Exam: 40 Marks

Course Outcome: After studying this course, the students will an understanding

- Of bio elements and their compounds like metalloporpyrin and their role in biological system.
- ➤ Have an advanced knowledge of the role of different metalloenzymes in catalytic reactions in biological system.
- Have an understanding of beneficial and toxic effects of certain metals in certain forms and doses on life.

### 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. 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.

# **Unit-II** Biological Activity of Essential Trace Elements and Metallotherapy

### (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.

Copper in Biochemical systems: Electron transfer, oxidation and oxygenation of substrates.

Zinc in Biosystems: Lewis acid catalyst, Enzyme activator in vitamin B12.

Biochemical basis of essential metal deficient diseases and their therapies (Iron, Zinc, Copper and Manganese).

Metal complex as drugs: Platinum, Rhodium and Gold complexes.

Antibacterial, Antiviral and Antifungal activities of metal complexes with probable mechanism of action.

# **Books Recommended**

- 1. Bioinorganic Chemistry-A Survey; Ei- Ichiro Ochiai; Academic Press; 2008.
- 2. Bio inorganic Chemistry- An introduction; Ochiai; Allyn and Bacon; 1977.
- 3. Inorganic Biochemistry; Vol. 1&2; Eichhorn; Elsevier, 1973.
- 4. Inorganic Aspects of Biological and Organic Chemistry; Hanzilik; Academic Pub.; 1976.
- 5. The Inorganic Chemistry of Biological processes; 2nd edn.; Hughes; Wiley; 1973.
- 6. A Text book of Medicinal aspects of Bio inorganic Chemistry; Das; CBS; 1990.
- 7. The Biological Chemistry of Elements; Frausto de Silva; Williams; Clarenden; 1991.
- 8. Principles of Bio inorganic Chemistry; Lippard, Berg; Univ. Science Books; 1994.

# Course No: CH21002OE Title: Chemistry of Bio-Molecules (02 Credits)

#### Max. Marks: 50 Continuous Assessment: 10 marks

### **Duration: 32 Contact hours End Term Exam: 40 Marks**

Course Outcome: 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
- > To know the importance of micronutrients.

# Unit-I

# (a) 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

### (b)Lipids

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

### Unit-II

### (16 Contact hours)

(a) Proteins and Enzymes Proteins: 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. (b) 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.

# **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).
- 3. Lehninger's Principles of Bio-chemistry; D.L. Nelson; M.Cox Worth publications; 2000.
- 4. Introduction to Nucleic Acids and Related Natural Products; Ulbight; Oldborn Press.
- 5. Chemsitry of Natural Products; S.V. Bhat, B.A. Nagasampagi, M. Siva Kumar. Naroosa Publishing House; New Delhi.