

# Course Structure for P.G. Programme in Chemistry as per CBCS w.e.f. 2021

## SEMESTER-I

### 1. Core Courses (CR):

Course No.	Title	Contact hours/Week	No. of Credits
CH21101CR	Inorganic Chemistry	(03L + 01T)	04
CH21102CR	Organic Chemistry	(03L + 01T )	04
CH21103CR	Physical Chemistry	(03L + 01T )	04
CH21104CR	Environmental Chemistry & Analytical Monitoring.	(01L + 01T)	02

### 2. Discipline Centric Electives (DCE):

Course No.	Title	Contact hours/Week	No. of Credits
CH21105DCE	Laboratory Course in Chemistry -I	04 Lab Sessions of 03 hours each total 45 sessions	04
CH21106DCE	Symmetry & Group Theory	(01L + 01T)	02
CH21107DCE	IR, Raman & Electronic Spectroscopy	(01L + 01T)	02

### 3. Generic Electives (GE):

Course No.	Title	Contact hours/Week	No. of Credits
CH21001GE	Surfactants and their Applications	(01L + 01T)	02

### 4. Open Elective Courses (OE):

Course No.	Title	Contact hours/Week	No. of Credits
CH21001OE	Chemistry in Everyday Life	(01L + 01T)	02

## SEMESTER-II

### 1. Core Courses (CR):

Course No.	Title	Contact hours/Week	No. of Credits
CH21201CR	Inorganic Chemistry	(03L + 01T)	04
CH21202CR	Organic Chemistry	(03L + 01T )	04
CH21203CR	Physical Chemistry	(03L + 01T )	04
CH21204CR	Green Chemistry	(01L + 01T)	02

### 2. Discipline Centric Elective (DCE):

Course No.	Title	Contact hours/Week	No. of Credits
CH21205DCE	Laboratory Course in Chemistry -II	04 Lab Sessions of 03 hours each total 45 sessions	04
CH21206DCE	NMR & ESR Spectroscopy	(01L + 01T)	02
CH21207DCE	Solid State Chemistry	(01L + 01T)	02

### 3. Generic Elective Courses (GE):

Course No.	Title	Contact hours/Week	No. of Credits
CH21002GE	Metal Ions in Living Systems	(01L + 01T)	02

### 4. Open Elective Course (OE):

Course No.	Title	Contact hours/Week	No. of Credits
CH21002OE	Chemistry of Bio-molecules	(01L + 01T)	02

## **SEMESTER-III**

### **1. Core Courses (CR):**

<b>Course No.</b>	<b>Title</b>	<b>Contact hours/Week</b>	<b>No. of Credits</b>
CH21301CR	Selected Topics in Inorganic Chemistry	(03L + 01T)	04
CH21302CR	Organic spectroscopy and heterocyclic chemistry	(03L + 01T )	04
CH21303CR	Physical Chemistry	(03L + 01T )	04
CH21304CR	Non-Equilibrium Thermodynamics	(01L + 01T)	02

### **2. Discipline Centric Elective (DCE):**

<b>Course No.</b>	<b>Title</b>	<b>Contact hours/Week</b>	<b>No. of Credits</b>
CH21305DCE	Laboratory Course in Chemistry -III	04 Lab Sessions of 03 hours each total 45 sessions	04
CH21306DCE	Chromatographic Techniques	(01L + 01T)	02
CH21307DCE	Bio-Physical Chemistry	(01L + 01T)	02

### **3. Generic Elective (GE):-**

<b>Course No.</b>	<b>Title</b>	<b>Contact hours/Week</b>	<b>No. of Credits</b>
CH21003GE	Bio-Organic Chemistry	(01L + 01T)	02

### **4. Open Elective Course (OE):**

<b>Course No.</b>	<b>Title</b>	<b>Contact hours/Week</b>	<b>No. of Credits</b>
CH21003OE	Medicinal Inorganic Chemistry	(01L + 01T)	02

## SEMESTER-IV

### 1. (i) Core Courses (CR):

Course No.	Title	Contact hours/Week	No. of Credits
CH21401CR	Advanced Inorganic Chemistry	(03L + 01T)	04
CH21402CR	Advanced Organic Chemistry	(03L + 01T)	04
CH21403CR	Advanced Physical Chemistry	(03L + 01T)	04
CH21404CR	Project Seminar and Dissertation	(01L + 01T)	02

### 2. Discipline Centric Electives (DCE)\*\*:

Course No.	Title	Contact hours/Week	No. of Credits
CH21405DCE	Lab Project in Chemistry	05 Lab Sessions of 03 Hours.	04
CH21406DCE	Inorganic Materials	(01L + 01T)	02
CH21407DCE	Supramolecular Chemistry	(01L + 01T)	02
CH21408 DCE	Medicinal Chemistry	(01L + 01T)	02
CH21409 DCE	Chemistry of Natural Products	(01L + 01T)	02
CH21410 DCE	Computational Chemistry and Advanced Quantum Chemistry	(01L + 01T)	02
CH21411DCE	Applied Electrochemistry	(01L + 01T)	02

Course No.	Title	Contact hours/Week	No. of Credits
CH21004GE	Synthetic Polymers and their Applications	(01L + 01T)	02
CH21005GE	Novel Materials	(01L + 01T)	02

### 3. Open Elective (OE):

Course No.	Title	Contact hours/Week	No. of Credits
CH21004OE	Food Chemistry	(01L + 01T)	02

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*Students in 4<sup>th</sup> semester have to necessarily opt for two DCE courses offered by the same specialization to have the higher credit weightage from a particular specialization.*

**Course No: CH21101CR**  
**Title: Inorganic Chemistry (04 Credits)**

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

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

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

- Know about the thermodynamic stability of metal complexes and learn the stepwise formation of complexes and their stability constant.
- Discuss the properties of coordination compounds and explain bonding in Octahedral, Square-planar and Tetrahedral complexes using Molecular Orbital Theory.
- Familiarize students about synergic nature of bonding in metal carbonyl complexes and the nature of interaction in other  $\pi$ -acceptor ligands.
- Understand the properties of Lanthanide elements and their complexation with different ligands and their applications.

**Unit-I Metal-Ligand Equilibria in Solution (16 Contact hours)**

Stepwise and overall formation constants (normal and abnormal trends). Mechanisms of selected Complexation processes, Inert & labile complexes.  $d^n$  configuration and lability, Stability of uncommon oxidation states. Metal Chelates: Characteristics, Chelate effect and the factors affecting stability of metal chelates. Ligand preorganization, Macrocyclic effect. Complexes of Crown ethers and Cryptands, Tertiary phosphine as ligand. Determination of formation constants by pH-metry and spectrophotometry. Structural (ionic radii) and thermodynamic (hydration and lattice energies) effects of crystal field splitting. Jahn-Teller distortion, spectrochemical series.

**Unit-II Bonding Models in Coordination Compounds: (16 Contact hours)**

Evidence of covalent bonding in transition metal complexes (Experimental Evidence in favor of Metal Ligand Orbital Overlap); Adjusted crystal field theory. Molecular orbital theory of bonding in octahedral complexes:- composition of ligand group orbitals; molecular orbitals and energy level diagram for sigma bonded  $ML_6$ ; Effect of pi bonding. (Pi donor and Acceptor Ligands). Molecular orbital and energy level diagram for bonding in Square-planar and Tetrahedral complexes.

**Unit-III Bonding in Pi-acid Metal Complexes and Chelation Therapy (16 Contact hours)**

Transition Metal Carbonyls: Carbon monoxide as Pi acid ligand, structure and bonding of mono- and poly-nuclear carbonyls. Spectroscopic characterization (Vibrational spectra) of metal carbonyls. Structure and bonding of transition metal nitrosyls, dinitrogen and dioxygen complexes.

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

**Unit-IV Coordination Chemistry of Lanthanides (16 Contact hours)**

Electronic Configuration and Oxidation states. f-orbital's. Coordination numbers, stereochemistry and stability of lanthanide Complexes. Selected examples of lanthanide complexes with nitrate,  $\beta$ -Diketonate, crown Ether and porphyrin type ligands. Homo and hetero dinuclear coordination compounds, coordination polymers of lanthanide ions.

Properties and Applications of Lanthanides: General Overview. Utility of Lanthanide Complexes as Sensory Probes, Lasers, NMR Shift Reagents and Contrast Agents in Magnetic Resonance Imaging (MRI). lanthanide Single molecule magnets

***Books Recommended:***

1. Lanthanide and Actinide Chemistry; Simon Cotton; 2<sup>nd</sup> Revised Edn.; John Wiley & Sons: West Sussex, England; 2006.
2. Inorganic Chemistry; Weller, Overton, Rourke, Armstrong; 6<sup>th</sup>Edn.; Oxford University Press; 2017 Reprint
3. Inorganic Chemistry; G. Wulfsberg; Viva Books Private Limited; 2005 Reprint
4. Chemistry of the Elements; 2<sup>nd</sup>Edn; N. N. Greenwood, A. Earnshaw; Elsevier; 2014 Reprint
5. Inorganic Chemistry; 3<sup>rd</sup>Edn; D. F. Shriver; P. W. Atkins; Oxford; 1999.
6. Advanced Inorganic Chemistry; Vol-1, 34<sup>th</sup> Reprint 2013; Krishna Educational Publishers
7. Concise Inorganic Chemistry; J. D. Lee; 5<sup>th</sup>Edn.; Black Well Publishing; 2006
8. Books Recommended
9. Principles of Inorganic Chemistry; 1st edn.; Brain W. Pfennig; Wiley; 2015.
10. Advanced Inorganic Chemistry; 5th and 6th edn; F.A. Cotton , G. Wilkinson; Wiley;1998/1999.
11. Inorganic Chemistry; 4th edn; J. E. Huheey; E. A. Keiter; Harper Collins; 2009.
12. Inorganic Chemistry; G. Wulfsberg; Viva; 2002.
13. Chemistry of the Elements; 2nd edn; N. N. Greenwood, A. Earnshaw; Butterworth; 1997.
14. Inorganic Chemistry; 3
15. rdedn; D. F. Shriver; P. W. Atkins; Oxford; 1999.
16. Inorganic Chemistry; K.F. Purcell, J.C Kotz; Saunders; 1977.
17. Coordination Chemistry; D. Banerjea; Tata McGraw Hill; 1993 .

**Course No: CH21102CR**  
**Title: Organic Chemistry (04 Credits)**

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

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

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

- Recognize the key reactive intermediates their stability and determination of reaction mechanism.
- Grasp different aspects of stereochemistry.
- Understand the different types of substitution reaction mechanisms in both aliphatic and aromatic compounds and elimination reactions.

**Unit-I: Basic Organic Chemistry and Reactive intermediates (16 Contact hours)**

**Recapitulation of basic concepts:** Inductive effect. Concept of hybridization. Orbital pictures of bonding in C-C, C-N & C-O systems involving  $sp^3$ ,  $sp^2$  and  $sp$  hybridizations. Conjugation, Cross conjugation, Resonance, Rules for writing resonance structures. Hyperconjugation– Isovalent and sacrificial hyperconjugations. Concept of acids and bases and factors affecting acidity and basicity. Nucleophiles and Electrophiles. Tautomerism.

**Aromaticity:** Huckel rule and concept of aromaticity, Molecular orbital diagram of annulenes, Frost diagram. Relation between NMR and aromaticity. Anti and Homoaromaticity  
**Annulenes:** Systems with  $\pi$ -electron numbers other than six (2,4,8,10 and more than ten  $\pi$ -electron systems), Aromaticity of hetero annulenes. Aromaticity in fused ring systems. Aromaticity of ferrocene and azulene. Carcinogenesis due to aromatic hydrocarbons.

**Types of Reaction Mechanism:** Ionic, Radical and Pericyclic. Heterolytic bond cleavage and heterogenic bond formation. Homolytic bond cleavage and homogenic bond formation. Arrow formalism.

**Reactive Intermediates:** Generation, Structure, fate and stability of Carbocations (Classical and Non- Classical), Carbanions, Free radicals, Carbenes, Nitrenes, Arynes and Radical ions.

**Unit-II: Physical Organic Chemistry and Reaction Mechanism-I**

**(16 Contact hours)**

**Determination of Reaction Mechanism:** Reaction coordinate diagrams. Thermodynamic and kinetic evidences. Transition states & Intermediates (Hammond postulate). Structure of Product. Isotope effects – primary and secondary isotope effects. Isotope labeling, double labelling and kinetic isotope effects. Experiments for identifying mechanism (example of Cannizzaro reaction), product and intermediate identification, common intermediate detection, trapping and competition experiments, crossover experiments. Stereochemical evidence. Specific and general acid and base catalysis.

**Aliphatic Nucleophilic Substitutions:** Mechanism, stereochemical implications and comparison of  $S_N2$ ,  $S_N1$ ,  $S_Ni$  and NGP reactions. Factors affecting rates of  $S_N1$  and  $S_N2$  reactions. Nucleophilic substitution at allylic, benzylic, aliphatic trigonal and vinylic carbons. Mitsunobu reactions. Nucleophilic substitutions on elements other than carbon. Examples of nucleophilic substitutions in biological systems.

**Elimination reactions:** Mechanism and stereochemical implications of E1, E2, E1cB and E2C elimination reactions. Factors affecting these reactions. Competition between substitution and elimination reactions. Elimination in cyclic systems and vinyl halides. Mechanism and orientation in pyrolytic eliminations, Shapiro reaction.

### Unit-III: Reaction Mechanism-II

(16 Contact hours)

**Aliphatic Electrophilic Substitutions:** General mechanism of  $S_E1$ ,  $S_E2$  and  $S_Ei$  reactions. Stork-Enamine reaction.

**Aromatic Electrophilic Substitution:** General mechanism and Energy profile diagram. Orientation and reactivity in mono substituted benzene ring, Ortho / Para ratio. The third substitution. Ipso attack. Reversal of F.C. alkylation. Synthetic application of F.C. acylation and nitration reactions (Toluene to nitro – benzoic acids, synthesis of ortho & Para nitro anilines).

**Aromatic Nucleophilic substitution:** Discussion of different mechanisms ( $S_N1$ ,  $S_NAr$ , Benzyne and  $S_{RN}1$ ). Mechanisms of Von- Richter, Sommelet-Hauser and Smiles rearrangements and Chichibabin reaction.

**Free Radical Substitution:** Free radical substitution mechanisms. Neighbouring Group Assistance in free radical reactions. Factors affecting radical substitutions. Auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sandmeyer and Hunsdiecker reactions.

### Unit-IV: Stereochemistry of Organic Compounds

(16 Contact hours)

**Stereoisomerism:** Classification, molecules with one, two or more chiral centres; Configuration nomenclature, D L, R S and E Z nomenclature. Axial and planar chirality and helicity (P & M); Stereochemistry and configurations of allenes, spiranes, alkylidene cycloalkanes, adamantanes, catenanes, biphenyls (atropisomerism), bridged biphenyls, ansa compounds and cyclophanes. Racemic modification.

**Topicity and prostereoisomerism:** Topicity of ligands and faces and their nomenclature; Stereogenicity, chirogenicity, and pseudoasymmetry, stereogenic and prochiral centres. Simple chemical correlation of configurations with examples, quasiracemates.

**Cyclostereoisomerism:** Configurations, conformations and stability of cyclohexanes (mono-, di-, and trisubstituted), cyclohexenes, cyclohexanones, halocyclohexanones, decalins, decalols and decalones.

**Asymmetric induction:** Dynamic stereochemistry (acyclic and cyclic), Qualitative correlation between conformation and reactivity, Curtin-Hammett Principle.

#### ***Books Recommended:***

1. March's Advanced Organic Chemistry Reactions, Mechanism and Structure, 6<sup>th</sup> Ed., 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 Revised Ed., 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).
7. 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. Stereochemistry of Organic Compounds 2<sup>nd</sup> Ed., D. Nasipuri. (New Age Inter.- 2008)
11. Stereochemistry of Carbon Compounds - E.L.Eliel. (TMH -2007)
12. Stereochemistry of Organic Compounds 7<sup>th</sup> Ed. - P.S. Kalsi. (New Age Inter.- 2012).

**Course No: CH21103CR**  
**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:

- be able to understand the genesis of quantum mechanics and its basic formulations for understanding the microscopic world.
- learn to solve the Schrodinger equation to evaluate energy of simple systems with or without potential energy.
- be able to appreciate the special physicochemical aspects and implications of solid-liquid, liquid-liquid and liquid-air interfaces.
- learn what are fast reactions and how kinetic investigations are carried out for such reactions.
- understand why chemical reactions are associated with energy barriers
- learn about the basic approximations, and theoretical predictions from different reaction rate theories like collision theory, transition state theory, theories of unimolecular reactions and linear free energy relations.
- be able to make predictions about the rate constants of reactions using different reaction rate theories and free energy relations and compare the same with experimental data
- be able appreciate the need and role of solvent in chemical reactions
- learn about the basic and applied aspects of surface and enzyme catalyzed reactions

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

**Exact quantum mechanical results:** Time-independent and time-dependent Schrodinger equation. Postulates of quantum mechanics. Operator concept, quantum mechanical operators in Cartesian and Spherical polar co-ordinate systems, some properties of quantum mechanical operators. Review of particle in a box problem. The solution of problems of harmonic oscillator & the rigid rotator. Tunneling effect.

Born-Oppenheimer approximation. Solution of the Hydrogen-like atom problem, radial and angular wave functions.

**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.

**Thermodynamics of Interfaces:** Surface excess, surface tension and thermodynamic parameters, Gibbs adsorption isotherm.

**Solid liquid interface:** Contact angle, young's equation, wetting, Wetting as contact angle phenomena.

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

**Unit-III Chemical kinetics-I** **(16 Contact hours)**

**Overview of basic concepts:** Macroscopic and microscopic kinetics, kinetic analysis of experimental data, Differential method, integration method.

**Fast reactions:** General features of fast reactions, study of fast reactions by flow method, relaxation method and flash photolysis.



**Theories of Chemical Reactions:** Overview of Arrhenius and Collision theory, Potential energy surfaces, Activated complex theory of reaction rates, statistical & thermodynamic formulations, comparison with collision theory.

**Unimolecular reactions:** Lindman, Hinshelwood, RRK and RRKM theories.

**Structure Reactivity Relationships:** Quadratic Free-Energy Relationships (QFER), Hammett and Taft relationships.

#### **Unit-IV Chemical kinetics-II**

**(16 Contact hours)**

**Surface Reactions:** Unimolecular & bimolecular surface reactions [Langmuir-Hinshelwood & Langmuir-Riedel mechanism], classical & statistical treatments.

**Reactions in solutions:** Effect of solvent on reaction rates, Diffusion controlled reactions (partial & full microscopic diffusion control), Ionic Reactions; Single & double sphere models of ionic reactions, effect of ionic strength.

**Enzyme catalyzed Reactions:** Kinetics of enzyme catalyzed reactions, Effect of substrate concentration, temperature and pH. Enzyme inhibition.

**Chain reactions:** Explosive reactions, Polymerization reactions (free radical, cationic and anionic)

#### **Books Recommended:**

1. Physical Chemistry –P. W. Atkins, 9th Edition, ELBS, Oxford, 2009.
2. Physical Chemistry- A Molecular Approach - D. A. McQuarrie & 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. 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. Chemical Kinetics, K. J. Laidler, 3rd Edition, Pearson, 1987.
9. Chemical Kinetics and Reaction Dynamics, Paul L. Houston, Dover Publications, INC., Mineola, New York, 2001.
10. Chemical Kinetics and Dynamics, J. I. Steinfeld, J. S. Francisco, W.L. Hase, Prentice Hall, 1989
11. Chemical Kinetics and Catalysis, R.I. Masel, Wiley, 2001
12. Chemical Kinetics: From Molecular Structure to Chemical Reactivity, Luis G Arnaut, Sebastiao Jose Formosinho, Hugh Burrows, Elsevier, 2007.

**Course No: CH21104CR**

**Title: Environmental Chemistry and Analytical Monitoring (02 Credits)**

**Max. Marks: 50**

**Continuous Assessment: 10 marks**

**Duration: 32 Contact hours**

**End Term Exam: 40 Marks**

**Unit-I Chemistry of the Environment (16 Contact hours)**

**Atmosphere:** Vertical profile of the atmosphere; troposphere reactivity patterns; stratospheric chemistry (Chapman mechanism and ozone depletion).

Chemistry and control of Green house effect, Acid rain and Photochemical smog.

**Hydrosphere:** Factors determining composition of water bodies (acid-base, Distribution diagram), thermal-stratification, pE concept and Pourbaix diagram and oxygen sag curve).

Chemistry of water treatment: Chlorination, Ozonation and UV radiation.

Water treatment techniques: adsorption and Photo catalysis by Nanomaterials.

**Unit-II Analytical Environmental Monitoring (16 Contact hours)**

Analytical methods for measuring air pollutants: General aspects, Sampling and methods of analyses. Water quality parameters: Dissolved oxygen, metals (As, Cd, Hg, Pb and Se), chloride, phosphate and nitrate. Water quality standards. Continuous monitoring instruments as analytical tools for realtime monitoring of pollutants (NDIR, GC-MS, Chemiluminescence and Spectrophotometry).

Water Analysis Methods: Classical, Spectrophotometry (Chromogenic step), Electrochemical methods and Ion-chromatography.

Analytical methods for determining dissolved oxygen, BOD and COD. Choice of methods for determining trace metals (As, Cd, Hg, Pb and Se)

***Books Recommended***

1. Environmental Chemistry; Nigel J. Bunce; Wurez Publishers; 1991.
2. Environmental Chemistry; 2<sup>nd</sup> edn; Colin Baird; Freeman & Co; 1991.
3. A Textbook of Environmental Chemistry; O.D. Tyagi & M. Mehra; Anmol Publishers; 1990.
4. Environmental Chemistry; A. K. De; Wiley Eastern; 1995.
5. Environmental pollution Analysis; S.M. Khopkar; Wiley Eastern.
6. Environmental Chemistry; S.E. Manahan (6<sup>th</sup> / 7<sup>th</sup> / 8<sup>th</sup> / 9<sup>th</sup> Edns); Lewis Publishers.
7. Environmental pollution; B.K. Sharma & H. Kaur; Goel Publishers; 1996.

**Course No: CH21105DCE**  
**Title: Laboratory Course in Chemistry-I (04 Credits)**

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

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

**Course Outcomes:** The course is elementary and fundamental for the new M. Sc. Students and involves experiments from Inorganic, Organic and Physical chemistry. The students will get an opportunity to plan and conduct their experiments individually and rich theoretical appraisal of the experiments will help students to understand applications and relevance of chemistry.

**SECTION A- INORGANIC CHEMISTRY**

**I. Synthesis and Characterization of the Coordination Compounds of Transition metals.**

- A. Theoretical appraisal of first row Transition metal Coordination Chemistry.
- B. Synthesis as a Laboratory Technique (Concepts, Calculations and Design of Synthetic procedures).
- C. Selected preparations of the following coordination compounds with the specific objectives:

***1 Trithioureacopper(I)sulphate monohydrate:***

- i) Electron-neutrality Principle, ii) In-situ generation and Stabilization of unusual oxidation state, iii) Purification by recrystallization, iv) Observation of crystal morphology under microscope and v) Characterization through thermal (M.P., TGA and DTA) and spectroscopic (FT-IR and DR-UV-Vis) methods.

***2 Trisethylenediaminecobalt(III) chloride:***

- i) Stabilization of Unusual Oxidation state, ii) Redox Chemistry of Co(II)/Co(III), iii) Resolution of racemic mixture, iv) Characterization through thermal methods (M.P., TGA and DTA) Spectroscopic methods (FT-IR and DR-UV).

**II. Inorganic Quantitative Analyses.**

**A. Gravimetry:**

- i) Skill and importance of weighing in Chemistry, Gravimetric Calculations
- ii) Precipitation process in homogenous mixtures, Precipitating agents, conditions of precipitation.
- iii) Precipitate processing (Digestion, Ignition); reducing precipitation errors (Co- and post precipitation)

**B. Titrimetry:**

- i) Types and skill of titration, concept of Complexometric titrations, titrimetric calculations. ii) Metallochromic Indicators: selection, structure, and mechanism of action. iii) Role and selection of buffers in Complexometric titrations, EDTA Back titrations.

**C. Separation and estimation of following Binary metal ion systems using Gravimetry & Titrimetry simultaneously:**

- i) Silver ( $\text{Ag}^+$ ) as  $\text{AgCl}$  and Nickel ( $\text{Ni}^{2+}$ ) as  $[\text{NiEDTA}]^{2-}$  complex.
- ii) Nickel ( $\text{Ni}^{2+}$ ) as  $\text{Ni}(\text{DMG})$  complex and Magnesium ( $\text{Mg}^{2+}$ ) as  $[\text{MgEDTA}]^{2-}$  complex.
- iii) Copper ( $\text{Cu}^{2+}$ ) as  $\text{CuSCN}$  and Magnesium ( $\text{Mg}^{2+}$ ) as  $[\text{MgEDTA}]^{2-}$  complex.

**III. Paper Chromatography**

- (i) Principle, Separation process, Technique of Paper Chromatography. Design of mobile phase.
- (ii) Methods of paper chromatography (Ascending, Descending and Radial)

- (iii) Comparative mobile phase study of separating mixtures. Chromatogram analysis and Interpretation.

*Abbreviations Used: M.P. Melting Point, TGA Thermo-gravimetric analyses, DTA Differential thermal analyses, FT-IR Fourier Transform Infrared, DR-UV-Vis Diffuse Reflectance Ultraviolet-Visible, EDTA Ethylene diammine tetraacetate, DMG Dimethyl glaxymate, SCN thiocyanate.*

## **SECTION B- ORGANIC CHEMISTRY**

### **1. Qualitative Analyses of Organic Compounds**

- (I) **Physical Properties:** Physical state, colour, odour, solubility behaviour and melting / boiling points.
- (ii) **Chemical Properties**
- (a) **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, thioureas, nitro compounds and hydrocarbons.
2. **Separation, Purification and identification of Organic compounds from a two-component mixture: Derivatization and recrystallization.**
3. **Quantitative Estimation of the following compounds**
- (a) **Glucose.**
- (b) **Glycine**

## **SECTION C- PHYSICAL CHEMISTRY**

### **A. Chemical Kinetics**

1. Determination of order of reaction between  $K_2S_2O_8$  and KI by Initial rates method using clock reaction.
2. Compare the effect of ionic strength on the rate constant of persulphate-iodide reaction and iodide-Fe(III) reactions using clock method.
3. Determination of the rate constant of inversion of cane sugar catalysed by HCl using polarimeter.

### **B. Viscometry**

1. Investigation of variation of viscosity with conc. and determination of unknown concentration and the radius of solute molecule by viscosity measurement.
2. Determination of Mol. Mass of a Polymer (Polyvinyl alcohol) using viscosity method.

### **C. Calorimetry**

1. Determination of heat of neutralisation of a strong acid with a strong base.
2. Determination of heat of neutralisation of a weak acid with a strong base.

### **Books Recommended:**

1. Advanced Inorganic Chemistry, 5<sup>th</sup>ed. / 6<sup>th</sup>ed., F.A. Cotton , G. Wilkinson ; Wiley 1998/1999
2. Coordination Chemistry - D. Banerjea ; Tata McGraw Hill, 1993.
3. Vogel's Textbook of Quantitative chemical Analysis; 5<sup>th</sup>edn; Jeffery, Bassett; (ELBS, 1989).
4. Quantitative Analysis; 6<sup>th</sup>edn; Day, Underwood (Printice Hall, 1993).

5. Analytical Chemistry, 6<sup>th</sup>Ed; D. Christian, Wiley.
6. Quantitative Analysis; 6<sup>th</sup>edn; Day, Underwood (Printice Hall, 1993).
7. Experiments and Techniques in Organic Chemistry - D. Pasto, C. Johnson and M. Miller (Prentice-hall, **1992.**)
8. Microscale and Macroscale Organic Experiments- K.L. Williamson (D.C. Heath and Co., **1989**).
9. Advanced Practical Organic Chemistry, 2nd ed. - N.K. Vishnoi (Vikas, **1999**).
10. Vogel's Textbook of Practical Organic Chemistry, 5th ed.- A.R. Tatchell (ELBS, • **1996**)
11. Comprehensive Practical Organic Chemistry, V. K. Ahluwalia and Renu Aggarwal, (University Press-**2000**).
12. Practical Physical Chemistry, Findley, Kitchener, Longman, 1977.
13. Advanced Practical Physical Chemistry, Yadav , Goel Pub, 1994.
14. Experiments in Physical Chemistry, 5th ed., Schoemaker et al. , MGH, 1989.

**Course No: CH21106DCE**  
**Title: Symmetry and Group Theory (02 Credits)**

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

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

**Course Outcome:** Molecular symmetry is of fundamental importance for understanding spectroscopy and crystallography, as well as molecular properties. The fundamental aspects (symmetry elements, their combination, and point groups) and applications (to electronic, infra-red, and Raman spectroscopy) are taught and students are expected to assign symmetry point groups, construct character tables, and apply the understanding to explain electronic, IR, and Raman behaviour of the molecules.

**Unit-I Molecular Symmetry (16 Contact hours)**

Molecular Symmetry - Symmetry elements and operations: Identity, rotation axis, reflection plane, inversion centre, improper rotation axis. Combination of symmetry operations, Introductory idea to permutation group. Group multiplication tables. Symmetry groups  
Symmetry Classification of Molecules: Point groups. Schoenflies notation of point groups. Identification of point groups. Matrices and their combination, block factored matrices, Matrix representation of symmetry operations.

**Unit-II Character Tables and Spectroscopy (16 contact hours)**

The Great Orthogonality Theorem-elementary idea, consequences of the Great Orthogonality Theorem. Reducible and Irreducible representations (IRs), Mulliken symbols for IRs, Properties of IRs. Character table-construction of character tables for  $C_{2v}$ ,  $C_{3v}$  and  $C_{4v}$  point groups.

Applications of group theory to IR and Raman spectroscopy. Degrees of freedom/molecular motions-Vibrational motions. Selection rules. Symmetry of IR and Raman active normal vibrational modes of  $AB_2$ ,  $AB_3$ ,  $AB_4$ ,  $AB_5$ , and  $AB_6$  type molecules.

Applications of symmetry to Molecular Chirality, Polarity and hybridization. Projection Operators (Elementary Idea)

**Books Recommended**

1. Chemical Applications of Group Theory; 2nd edn.; F.A.Cotton; Wiley Eastern; (1994)
2. Molecular Symmetry and Group Theory; L. Carter; Wiley; 1998.
3. Symmetry and Spectroscopy of Molecules; K. Veera Reddy; New Age 1998.
4. Inorganic Chemistry, Principles of structure and reactivity; 4th Edition; James E. Huheey, Ellen A. Keiter and Richard L. Keiter. Pearson Education Inc
5. Physical Methods for Chemists; R.S.Drago; 2nd edn; Saunders; 1992.

**Course No: CH21107DCE**

**Title: Infrared, Raman and Electronic Spectroscopy (02 Credits)**

**Max. Marks: 50**

**Continuous Assessment: 10 marks**

**Duration: 32 Contact hours**

**End Term Exam: 40 Marks**

**Course Outcomes:** This course is aimed to provide the basic and advanced level understanding about Electronic, Infrared and Raman spectroscopy to students of MSc 1st semester, from a Physico-Chemical perspective. The students are expected to learn the conceptual basis of the subject and trained in problem solving and applications to various chemical systems.

**Unit-I (a) Fundamentals of Spectroscopy (08 Contact hours)**

Interaction of light with matter, transition probability, transition moment integral, derivation of selection rules.

Intensity of spectral lines; Einstein's treatment of absorption and emission processes. Beer Lambert Law: Transmittance, Absorbance, Molar Integrated Intensity, Oscillator strength.

Natural spectral line width, broadening of spectral lines -Doppler and Collision effects.

**(b) Electronic and Photoelectron Spectroscopy (08 Contact hours)**

Electronic Spectroscopy: Vibronic transitions. Intensity of spectra—the Franck-Condon principle. Electronic spectra of organic molecules, chromophores, auxochrome, spectral shifts Different types of electronic transitions; nomenclature, symmetry labels of electronic states--spectra of formaldehyde, Symmetry selection rules, Term Symbol (Elementary Idea). Effects of solvent, electron withdrawing and electron donating groups, conjugation and extended conjugation on the position of spectral bands.

Photoelectron Spectroscopy: Basic principles- photoionization process; ionization energies; Koopman's theorem. Photoelectron spectra of simple molecules (N<sub>2</sub>, O<sub>2</sub>),

**Unit-II (a) Infrared Spectroscopy (08 Contact hours)**

Linear harmonic oscillator- classical and quantum treatment of vibrations, vibrational energies of diatomic molecules, zero point energy, force constant and bond strength, anharmonicity, Morse potential energy levels. Fundamental bands, overtones and hot bands. Vibration- rotation spectra of diatomic molecules; P, Q and R branches;

Vibrations of polyatomic molecules: Normal vibrational modes, selection rules; combination and difference bands. Factors influencing the band positions and intensities. Group frequencies and finger print region.

**(b) Raman Spectroscopy (08 Contact hours)**

Classical and Quantum theories of Raman scattering, Molecular polarizability, rotational, vibrational, and vibrational-rotational Raman spectra. Selection rules; rule of mutual exclusion. Applications.

### ***Books Recommended***

1. Molecular Spectroscopy; 2<sup>nd</sup>edn; J L. McHale; CRC Press 2015.
2. Infrared and Raman Spectroscopy; Principles and Spectral Interpretation; 2<sup>nd</sup>edn.; P. Larkin; Elsevier; 2011.
3. Introduction of Spectroscopy; 4<sup>th</sup>edn.; D.L. Pavia, G. M. Lampman, G.S.Kriz, J.Vyvan; Cengage Learning, 2008.
4. Introductory Raman Spectroscopy; J. R. Ferraro, K.Nakamoto & C. W Brown; 2nd edn; Academic Press 2005.
5. Modern Spectroscopy; J.M.Hollas; Wiley; 2004..
6. Physical Methods for Chemists; R.S.Drago; 2nd edn; Saunders; 1992.
7. Fundamentals of Molecular Spectroscopy; C.N.Banwell, E.M.Mc Cash; 4th edn; Tata McGrawHill; 1994.
8. Physical chemistry; P. W. Atkins; 6th edition; Oxford University Press; 1998.
9. Electronic Absorption Spectroscopy and related techniques; D N Sathyanarayna; UniversitiesPress.
10. Theory and Applications of Ultraviolet Spectroscopy; H.H.Jaffe, M.Orchin; Wiley; 1962.
11. Molecular Spectroscopy; 1<sup>st</sup>Edn; J.L. Mchale; Prentice Hall; 1999.
12. Structural Methods in Inorganic Chemistry; 2nd edn; E.A.V.Ebsworth, D.W.H.Rankin, S.Cradock; Blackwell; 1991.



**Course No: CH21001GE**  
**Title: Surfactants and their Applications (02 Credits)**

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

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

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

- be familiar with the types of surfactants, their aggregation behavior and structure of aggregates.
- be familiar with the applications of the surfactant systems in da-to-day life, industries, catalysis, environment and pharmaceuticals.

**Unit-I Surfactant and their properties (16 contact hours)**

- a) **Surfactants and Micelles** :Classification of Surfactants, Solubility of Surfactants: Kraft temperature and cloud point, Micellization of surfactants: critical micelle concentration (cmc), aggregation number, counterion binding, factors affecting cmc in aqueous media. Thermodynamics of micellization: pseudophase model and mass action models. Structure and shape of micelles: geometrical consideration of chain packing, variation of micellar size and shape with surfactant concentration.
- b) **Micellar Solubilization and Catalysis**: Introduction, factors affecting micellar solubilization: nature of surfactant/solubilizate, effect of additive and temperature. Effect of solubilization on micellar structure, cloud point and cmc of surfactants. Solubilization of drugs into micelles and its importance in drug delivery systems and controlled release. Theoretical consideration of reactions in micellar media. Examples of micellar catalysis for hydrolysis, oxidation and reduction reactions

**Unit-II Mixed Surfactant and Surfactant-polymer Systems (16 Contact hours)**

- a) **Mixed Surfactant systems**: Mixed micelle formation, mixed monolayer formation, synergism, various models of mixed micelle formation(Clint and Rubingh) and mixed monolayer formation(Rosen's model). Importance and practical applications of mixed surfactant systems.
- b) **Surfactant-Polymer Systems**:Effect of polymers on aggregation behavior of surfactants and the factors governing their interaction. Phase behavior of polymer-surfactant mixtures. Surfactant-protein interaction: introduction, Applications of surfactant-polymers systems.

**Books Recommended**

1. Properties of Liquids and Solutions; J.N. Murell and E. H. Boucher; John Wiley & Sons Ltd; 1982.
2. Principles of Colloid and Surface Chemistry; P.C. Heimenz; Marcel Dekker Inc; New York; 1986.
3. Surfactants and Interfacial Phenomena; M. J. Rosen; John Wiley & Sons; New York; 1989.
4. Colloid and Interface Chemistry; R. D. Vold and M. J. Vold; Addison-Wesley; 1982.
5. Surfaces, Interfaces and Colloid; D. Y. Meyer; VCH Publishers; Inc; 1991.
6. Surfactants and polymers in aqueous solution; Jonsson, Lindmann, Homberg and Kronberg; John Wiley and sons; 1998.
7. Advances in Colloid and Polymer Science; B.K.Paul&S.P.Moulik, Current Science,Vol.80,p 990-,2001; Vol.78,p 99,1998.
8. Critical Reviews in Food Science and Nutrition; John Flanagan & Harjinder Singh, ,Vol. 46, pp221-237, 2006.
9. Drug Delivery Reviews; M. J. Lawrence &G.D.Rees; Vol, 45, p 898, 2000.

**Course No: CH21001OE**  
**Title: Chemistry in Everyday Life (02 Credits)**

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

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

**Course outcomes:** On completion of the course, the students will acquire knowledge of:

- Chemistry involved in Water & its different methods of treatment.
- Different household chemicals like Soaps, Detergents, Optical Brighteners, Shampoos etc.
- Different types of Polymers used in day to day life.
- Chemistry of Oils and Gases.

**UNIT-I (a) Water- An Amazing Chemical Stuff (16 contact hours)**

Molecular structure and its unique properties. Composition of natural water. Hard and Soft water. Standards for drinking water. Major causes of water pollution. Methods of treatment of water for domestic purposes including Reverse Osmosis.

**(b) Household Chemicals**

Chemistry of Soaps, Detergents, Optical Brighteners and Bleaching agents, Shampoos, Conditioners, Dyes, Hair Curling and Permanents, Deodorants and Antiperspirants, Perfumes, Tooth Pastes and Sunscreen Lotions. Disinfectants and moth repellents.

**Unit-II: (a) Polymers and Plastics: (16 contact hours)**

Characteristics and Types of Polymers. The big six of Polymer: Low Density Polyethylene (LDPE), High Density Polyethylene (HDPE), Polypropylene (PP), Polystyrene (PS), Polyvinyl Chloride (PVC) and Polyethylene - Tetra phthalate (PET or PETE)- their chemical characteristics and uses.

**(b) Oil & Natural Gases**

Composition & Chemical structures of Petroleum Products. Refining of Petroleum, Cracking & Catalytic Reforming. Octane & Cetane rating of fuels. Diesel engine fuel, Kerosene and Gasoline. Lead in Petrol: Its role, disadvantages & alternatives. LPG & CNG as fuel. Addition of mercaptanes to Natural gases for safety reasons.

***Books Recommended***

1. Principles of Modern Chemistry; 2nd edn; Oxtoby and Nachtrieb; Saunders College Publications; 1987.
2. Chemistry Fundamentals An Environmental Perspective; 2nd edn; Buell and Girard; Jones and Barlett; 2013.
3. [www.chemistryincontext.org](http://www.chemistryincontext.org); (American Chemical Society)

**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  $n_{Pt}^{\circ}$  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)**

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:** **(16 Contact hours)**

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 (16 Contact hours)**

**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 (14 Contact hours)**

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, Demjanov, Benzil-Benzilic acid, Favorskii, Arndt-Eistert, Neber, Hofmann, Curtius, Lossen, Schmidt, Beckmann, Baeyer-Villiger, Pyne and Dienone - phenol rearrangements.

**Unit-III Photochemistry (20 Contact hours)**

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-Loefer-Freytag reactions.

#### **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 Antarafacial 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 Antarafacial shifts of hydrogen atom.

#### ***Books Recommended***

1. March's Advanced Organic Chemistry Reactions, Mechanism and Structure, 6th Ed., 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 Revised Ed., 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).
7. 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 (16 Contact hours)**

**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 to hydrogen 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 (16 Contact hours)**

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:  $CHCl_3$ - $CH_3COOH$ - $H_2O$ ,  $NH_4Cl$ - $(NH_4)_2SO_4$ - $H_2O$  and Pb-Bi-Sn systems. First and second order phase transitions.

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

**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.

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, statistical mechanics 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. McQuarrie & 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 Green Chemistry. 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, Aqueous reaction conditions, Immobilized Solvents and irradiative reaction conditions. Examples of Green materials, reagents and some specific reactions.

**Unit-II Green Reactions (16 Contact hours)**

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). Green reactions involving synthesis of heterocyclic 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; 2nd Edn.; 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)**

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

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

**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.
- To know about conductometric Titrations

**SECTION A-INORGANIC CHEMISTRY**

**A: -Multi stage Inorganic Preparations:** (Any 03 Experiments)

- Preparation of tetraamminecarbonatocobalt (III) nitrate and its conversion to pentaamminechlorocobalt(III)chloride.
- Preparation of Trans-dichlorobis(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 Potassiumtrioxalatoferate(III)trihydrate and its component analysis.
- Preparation of Pentaamminechlorocobalt(III) chloride and study of Linkage isomers by its conversion to pentaamminenitritocobalt(III) chloride and to nitro isomer followed by IR Characterization.

**B: - Potentiometric Titrations:** (Any 03 Experiments)

- 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  $\text{AgNO}_3$  over Pt & Calomel assembly using  $\text{I}^- / \text{I}_2$  redox couple involving pseudo indicator action.
- Complexometric titration for determination of Ferro cyanide with standard Zinc (II) solution in order to establish the composition of the complex  $\text{K}_2\text{Zn}_3[\text{Fe}(\text{CN})_6]_2$

**C. pH-metric Titrations:** (Any 1 Experiment)

- Quantitative analysis of Chromate Dichromate mixture by pH Titration.
- Study of pH influence on a pH dependent redox reaction.

**D: - Conductometric Titrations:** (Any 1 Experiment)

- Conductometric investigation of Silver(I) ethylenediamine complexation reaction.
- Conductometric analysis of a strong binary acid mixture ( $\text{HNO}_3$  and  $\text{H}_2\text{SO}_4$ )

**SECTION B-ORGANIC CHEMISTRY**

1. **Separation, Purification and identification of Organic compounds from a three-component mixture**
2. **Organic Preparations**
  - (a) Bromination of Acetone using NBS & PTS
  - (b) Amidation Reaction
  - (c) Acetylation Reactions
  - (d) Haloform reaction: Preparation of Iodoform.

- (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. Conductometry**

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<sub>2</sub> and K<sub>2</sub>SO<sub>4</sub>/ (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>
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. Comprehensive 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., Schoemaker et 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 (16 Contact hours)**

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 (T<sub>1</sub>, T<sub>2</sub>). 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 – <sup>13</sup>C, <sup>19</sup>F and <sup>31</sup>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<sub>2</sub><sup>•-</sup>, CH<sup>•</sup>, BH<sup>•</sup> and F<sup>•-</sup>.

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.
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 Publishing 1983,
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**  
**Continuous 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; Clarendon; 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

Duration: 32 Contact hours

Continuous Assessment: 10 marks

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

(16 Contact hours)

##### (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, I.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.



**Course No: CH21301CR**  
**Title: Selected Topics in Inorganic Chemistry (04 Credits)**

**Max. Marks: 100**

**Continuous Assessment: 20 marks**

**Duration: 64 Contact hours**

**End Term Exam: 80 Marks**

**Course Outcome:** The students are expected:

- Learn the importance of inorganic elements in vital systems
- Discuss 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.
- To know about magnetic properties of the transition metal ions.
- Identify molecular geometries associated with various d-orbital splitting patterns
- Predict electron configurations of split d orbitals for selected transition metal atoms or ions
- Explain spectral and magnetic properties in terms of CFT concepts

**Unit-I Biological Inorganic Systems:**

**(16 Contact hours)**

**Iron Storage, Transport and Oxygen carriers:** Ferritin and Transferrin: Structure, Metal binding sites; incorporation and release of iron.

Haemoglobin and Myoglobin: Structure, oxygen saturation curves; Mechanism of oxygen transport and storage. Bohr Effect and cooperativity in haemoglobin. Dioxygen binding to Hemerythrin and Hemocyanin. Synthetic oxygen carrier model compounds: Vaska's iridium complex: Cobalt complexes with micro and macrocyclic ligands and Schiff base ligands.

Electron Carriers: Structure and biological role of Rubredoxin & Ferridoxin, Cytochromes as electron transfer proteins: structure, biological role and applications.

Biological Nitrogen Fixation: Nitrogenase enzyme; Fixation via nitride formation.

**Unit-II Bonding models in Inorganic Compounds**

**(16 Contact hours)**

**A. Bonding in main group compounds:** Classification and topology of Boron clusters, types of bonds, isolobal analogy, empirical rules for bonding in boron clusters, Selected examples of bonding in higher boranes; Carboranes and Metallacarboranes.

Bonding in Boron-Nitrogen, Phosphorous-Nitrogen and Sulphur-Nitrogen compounds ((Borazine, Cyclophosphazenes, phosphonitrilic halides, polythiazyls and Sulphur Nitrides) Bent's rule applications.

**B. Bonding in Metal clusters and Polymetallates:**

Factors favoring metal-metal bond, bonding in di- and trinuclear metal clusters, cotton rationale and quadruple bonding, selected examples of bonding in dinuclear metal clusters and hetero-polymetallates.

**C. Bonding in Metal Hydride Complexes:** Hydride as ligand, Characterization & Chemical reactions, Classical and Non classical Hydrides: Bonding and significance of Kuba's type Dihydrogen complexes.

### **Unit-III Magnetic Properties and Electronic Spectra of Transition Metal Complexes**

**(16 Contact hours)**

Types of magnetic behaviour, magnetic susceptibility and magnetic moment; methods of determining magnetic susceptibility; spin-only formula; L-S coupling, correlation of  $\mu_s$  and  $\mu_{\text{eff}}$  values; orbital contribution to magnetic moments; applications of magnetic moment data in investigation of nature of bonding and stereochemistry of first row transition metal complexes. High spin- low spin crossover. Magnetic Properties of Inner transition compounds.

Electronic spectra of Transition metal complexes: General features; Types of electronic transitions, theoretical aspects of d-d spectra, selection rules; spectral terms of  $d^1 - d^{10}$  metal ions.

Selected examples of d-d spectra. Spectra of distorted octahedral and square planar complexes. Charge transfer spectra (Factors affecting energies of LMCT and MLCT transitions).

### **Unit-IV NQR & Mossbauer Spectroscopy.**

**(16 Contact hours)**

**(a) Mossbauer Spectroscopy:** Basic principles, Nuclear Recoil and Mossbauer Effect, Spectral parameters such as isomer shift, quadrupole splitting and magnetic splitting, spectrum display. Determination of Magnetic transition Temperature, Intermediate spin -- Determination of Spin crossover temperatures. Partial Isomer shift and partial Quadrupole splitting. Application of the technique to the studies of (i) bonding and structure of  $\text{Fe}^{2+}$  and  $\text{Fe}^{3+}$  compounds (ii)  $\text{Sn}^{2+}$  and  $\text{Sn}^{4+}$  compounds— nature of M—L bond, coordination number and structure, (iii) detection of oxidation state and inequivalent MB atoms.

**(b) NQR Spectroscopy:** NQR isotopes, Nuclear quadrupole moment; Electric field gradient; nuclear quadrupole coupling constant; Axial Symmetry, Asymmetric EFG, Effect of applied magnetic field, Application

#### ***Books Recommended:***

1. Bioinorganic Chemistry- An introduction; Ochiai; Allyn and Bacon; 1977.
2. Principles of Bioinorganic Chemistry; S. J. Lippard and J. M. Berg; University Science Books; 1994.
3. The Inorganic Chemistry of Biological Processes; 2nd edn.; M. N. Hughes; John Wiley; 1973.
4. Bioinorganic Chemistry- A Short Course; R. M. Roat- Malone; Wiley Interscience; 2003.
5. Electronic Spectra of Transition Metal Complexes - D. Sutton (McGraw-Hill, 1968)
6. Elements of Magnetochemistry- R. L. Dutta, A. Syamal (Affiliated East -West, 1993).
7. Physical Methods for Chemistry; 2nd edn., R.S. Drago ; Saunders ; 1992.
8. Structural Methods in Inorganic Chemistry; 2nd edn. E. A. V. Ebsworth & D.W.H. Rankin; ELBS; 1991.
9. Spectroscopy in Inorganic Chemistry; Vols I & II; Rao, Ferraro; Academic; 1970.
10. NMR, NQR and Mossbauer Spectroscopy in Inorganic Chemistry; R.V. Parish; Ellis Horwood.

## Course No: CH21302CR

### Title: Organic Spectroscopy & Heterocyclic 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 will acquire knowledge of:

- IR range for functional groups,  $\lambda_{\text{max}}$  for polyenes and  $\alpha$ ,  $\beta$ -unsaturated carbonyl compounds which are helpful in structural elucidation of organic compounds.
- Fragmentation pattern in Mass spectrometry and its application in structural elucidation.
- Chemical shift values and their significance in NMR.
- Solving structural problems based on UV-Vis, IR,  $^1\text{H}$ NMR,  $^{13}\text{C}$ NMR and mass spectral data.
- Importance, structural properties and synthesis of Heterocyclic compounds with emphasis on monocyclic and bicyclic Heterocycles.

#### Unit I UV, IR AND Mass Spectroscopy

(16 Contact hours)

Principles and applications of Ultra Violet and Infra-Red Spectroscopy in structural elucidation of organic compounds.

**Mass Spectrometry:** Introduction, instrumentation, Ionization methods like EI, CI, SIMS, FAB, MALDI, ESI, MS/MS. Mass Analyzers like Magnetic Sector Mass Analyzer, Double Focusing Mass Analyzer, Quadrupole Mass Analyzer, Time-of-Flight. Determination of molecular formula, Role of Isotopes, Nitrogen Rule, Metastable Peak. Fragmentation pattern like Stevenson rule, initial ionization event,  $\alpha$ -cleavage, inductive cleavage, two bond cleavage, Retro-Diels. Alder cleavage, McLafferty Rearrangements. Fragmentation pattern of alkanes, alkenes, alcohols, phenols, aldehydes, ketones, Carboxylic acids, Amines, Problems based on Mass Spectrometry.

#### Unit II NMR Spectroscopy

(16 Contact hours)

Basic concepts, Mechanism of Measurements, Chemical shift values for various classes of compounds. Fourier Transform (FT), Techniques and advantages, Nuclear overhauser effect (NOE). One bond coupling, two bond coupling, three bond coupling, second order spectra A2, AB, AX, AB2, ABX, AX2, A2B2. Proton exchange, deuterium exchange, Peak broadening exchange C-13 NMR: Carbon 13-chemical shifts, proton coupled and decoupled spectra. Off-Resonance De-coupling, A quick dip into DEPT-45, DEPT-90, DEPT-135. Introduction to two-dimensional spectroscopy methods, Cosy techniques, HETCOR technique, OESY.

Structure elucidation of organic compounds using combined spectroscopic methods.

#### Unit-III Nomenclature, Structure and General Synthetic Methodologies

(16 Contact hours)

Nomenclature of heterocycles (Hantzsch- Widman and replacement methods). Non-aromatic and aromatic heterocycles. Tautomerism in heterocycles, Meso-ionic systems. Spectroscopic properties of heterocycles (IR, UV-Visible and NMR).

Reactions most frequently used in heterocyclic ring synthesis like C-C bonding, C-heteroatom bonding, typical reactant combinations, Electrocyclic processes in heterocyclic ring synthesis, Nitrenes in heterocyclic synthesis. Hantzsch Pyridine, Skraup, Fischer-Indole synthesis.

#### **Unit-IV Monocyclic and Bicyclic Heterocycles**

**(16 Contact hours)**

Structure, Synthesis and Reactions of Oxirane, Thirane, Azetidine, Pyrrole, Furan, Thiophene, Diazenes, Pyrimidines, Pyridine and Pyrans. Chemistry of five membered heterocycles with two heteroatoms like 1,3-Azoles, 1,2- Azoles.

Structure, Synthesis and reactions of Benzo-fused heterocycles like Benzo-pyrrole, Benzo-furan, Benzo-thiophene, Quinoline, Isoquinoline, Chromones and Coumarins.

#### ***Books recommended:***

1. Spectrometric Identification of Organic Compounds. 5th Ed., R. M. Silverstein, G. C. Bassler and T. C. Morill. (John Wiley-1991).
2. Introduction to NMR Spectroscopy, R. J. Abraham. J. Fisher and P. Loftus (Wiley-1991)
3. Applications of absorption spectroscopy of Organic Compounds, J. R. Dyer (Prentice Hall-1991).
4. Spectroscopic Methods in organic Chemistry, D. H. Williams; I. Fleming (Tata- McGraw Hill, 1988).
5. Heterocyclic Chemistry, 5<sup>th</sup> Ed. J.A.Joule and K.Mills, (Wiley-2010).
6. Essentials of Organic Chemistry, Paul M Dewick , (Wiley-2006).
7. Heterocyclic Chemistry, J.A. Joule and G.F.Smith , (Chapman and Hall-1996).
8. The Chemistry of Heterocycles Theophil Eicher and Siegfried Hauptmann, (George Thieme Verlag Stuttgart, New York -1995).
9. Heterocyclic Chemistry, Raj K. Bansal, (New Age International Publisher-2006).
10. Heterocyclic Chemistry, R. R. Gupta, M. Kumar, V. Gupta,(Springer-2006).

**Course No: CH21303CR**  
**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:

- learn quantum mechanical reason of the aromaticity and hybridization process in molecules.
- get acquainted with the multielectron wavefunction and evaluation of energy by using approximation methods in the multielectron systems.
- be familiar with the types of surfactants, their aggregation behavior and structure of aggregates.
- be familiar with the applications of the surfactant systems in industries, catalysis, environment and pharmaceuticals.
- learn how solvents influence the thermodynamic and transport properties of electrolyte solutions
- learn how different theories can be used for the quantification of thermodynamic and transport properties of electrolyte solutions
- have a know-how of the structural/electrical aspects of electrode/electrolyte interfaces and their impact over the thermodynamics and kinetics of charge transfer reactions across these interface
- learn about the basic mechanism underlying corrosion, factors affecting the rate of corrosion and different approaches for monitoring and control of corrosion of metals

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

**Chemical Bonding:** Hybridization of orbitals ( $sp$ ,  $sp^2$  &  $sp^3$ ). Huckel's Pi-MO theory: Application to linear and cyclic polyenes. Pi-electron charge and bond-order. Alternant hydrocarbons, Naphthalene, heteroatomic conjugated systems. Limitations of Huckel theory. Extended Huckel Method.

**Self consistent field method:** Hamiltonian and wave function for multi-electron systems. Electronic Hamiltonian, antisymmetrized wave function, Slater determinant. Hartree and Hartree-Fock self consistent field method. Application of HatreeFock SCF method to He-atom.

**Unit-II Self-Assembly of Surfactants and its applications (16 Contact hours)**

Classification of Surfactants, Solubility of Surfactants: Kraft temperature and cloud point, Micellization of surfactants: critical micelle concentration (cmc), aggregation number, counterion binding, factors affecting cmc in aqueous media. Thermodynamics of micellization: pseudophase model and mass action models. Structure and shape of micelles: geometrical consideration of chain packing, variation of micellar size and shape transitions with surfactant concentration, temperature and pH.

**Micellar solubilization:** Solubilization of hydrophobic molecules (like PAHs) in micelles, factors affecting micellar solubilization: nature of solubilizate and surfactant, effect of additive and temperature. Its applications in environmental remediation and oil recovery processes. Micelles as carriers of hydrophobic drug molecules and their pH and temperature responsive controlled release.

**Micellar catalysis:** Oxidation reduction reactions, micelles as scaffolds for effective energy transfer phenomena.

### **Unit-III Ionics**

**(16 Contact hours)**

**Ion solvent Interactions:** Non structural (Born) treatment and an introduction to structural (Ion-dipole, Ion-quadrupole) treatments of ion-solvent interactions.

**Ion-Ion Interactions:** Activity and activity co-efficient. Debye-Huckel theory of activity coefficients of electrolyte solutions; derivation of Debye-Huckel limiting law, validity and extension to high concentrations; ion-pair formation-Bjerrum model.

**Conductance of electrolyte solutions:** Mobility of ions, mobility and conductivity, Einstein relations, dependence of molar conductance on concentration, estimation of  $K$  and  $\Lambda_0$  for weak electrolytes, Theories of Conductance: Debye-Huckel-Onsager conductance equation and brief idea of its extension.

### **Unit-IV Electrodictics**

**(16 Contact hours)**

**Electrified Interface:** Metal-electrolyte electrified interface, concept of surface excess, thermodynamics of electrified interface, Lippman equation, electrocapillary curves. Methods for determination of surface excess.

**Structural models of metal-electrolyte interface:** Helmholtz-Perrin, Gouy-Chapman and Stern models, Structure of semiconductor/electrolyte interface.

**Theories of Heterogeneous Electron Transfer:** Electron transfer at electrified interface at and away from equilibrium. Butler-Volmer equation, low and high field approximations, significance of transfer coefficient, Marcus theory of charge transfer; basics and predictions.

**Electrodictics of Corrosion:** Corrosion, types and mechanism of corrosion, corrosion current, corrosion potential, Electrodictics of corrosion in absence of Oxide films, Corrosion and Evans diagrams, Monitoring and inhibition of corrosion; Cathodic and anodic protection, Passivation.

### **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. Molecular Thermodynamics of Electrolyte Solutions, Liloyd L Lee, World Scientific, 2008.
7. An Introduction to Aqueous Electrolyte Solutions, Margaret Robson Wright, Wiley, 2007.
8. Modern Electrochemistry 1, 2A, 2B 2nd Edition, J. O`M. Bokris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.
9. Electrochemical methods, Fundamentals and Methods, A.J. Bard, L.R. Faulkner, Wiley, 1980.
10. Physical Electrochemistry- Fundamentals, Techniques and Applications, Eliezer Gileadi, Wiley-VCH 2011.
11. Electrochemistry, 2nd Edition, Carl H. Hamann, Andrew Hammett, Wolf Vielstich, Wiley-VCH.

**Course No: CH21304CR**  
**Title: Non-Equilibrium Thermodynamics (02 Credits)**

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

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

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

- understand the concept of entropy production and learn how the extent of entropy production associated with different processes can be estimated
- learn about Onsager's formalism of irreversible processes and how it can be used to account how it can be used to explain various empirical relations observed in electrokinetic phenomena, Thermal diffusion, Thermomechanical effects and thermoelectric phenomena.
- learn how solvents influence the thermodynamic and transport properties of electrolyte solutions
- learn about some unique specialties of far-from-equilibrium systems like possible generation of order and symmetry breaking.

**Unit-I Fundamentals of Irreversible Thermodynamics (16 Contact hours)**

Basic principles of non-equilibrium thermodynamics: Second law of thermodynamics for open system, law of conservation of mass, charge and energy. Irreversible processes and uncompensated heat, degree of advancement, reaction rate & affinity, Relation of uncompensated heat to other thermodynamic functions.

Gibb's equation, entropy production, entropy production due to matter flow, heat flow, chemical reactions, charge flow; entropy production and efficiency of galvanic cells.

Concept of forces & fluxes, Onsager's theory of irreversible processes, phenomenological laws, their domain of validity. Principle of microscopic reversibility and Onsager relations, Chemical reactions near equilibrium. Curie-Prigogine principle. Transformation properties of forces and fluxes.

**Unit-II Applied Irreversible Thermodynamics (16 Contact hours)**

Stationary non-equilibrium states, thermodynamic significance. Theorem of minimum entropy production. States of minimum entropy production, stability of stationary states, entropy flow in stationary systems. Stationary state coupling in irreversible processes. Variation of entropy production in stationary states, Glansdroff-Prigogine inequality. Electrokinetic phenomena and expressions for streaming potential, electro-osmotic pressure difference, streaming potential using the linear phenomenological equations. Dufour and Soret effects, Thermal Osmosis, Thermo mechanical effects, thermoelectric phenomena.

Self-Organization in physico-chemical systems, Dissipative structures, thermal convection, Symmetry breaking in biological systems.

### ***Books Recommended***

1. Thermodynamics of Irreversible Processes; DeGroot, Mazur; Dover; 1986.
2. Introduction to Thermodynamics of Irreversible Processes; I. Prigogine; Wiley Interscience; 1967.
3. Thermodynamics for students of Chemistry, Kuriacose, Rajaram, (S. Chand and Co., 1996).
4. Exploring Complexity, I. Prigogine, G. Nicolis, (Freeman, 1998).
5. Molecular Thermodynamics, D. A. McQuarrie, J. D. Simon, USB, 1998.
6. Understanding non-equilibrium thermodynamics. G. Lebon, D. Jon, J. Casas Vasques. Springer, 2008.
7. Non-equilibrium thermodynamics, 2nd ed. Yasar Demirel. Elsevier, 2007.



## Course No: CH21305DCE

### Title: Laboratory Course in Chemistry III (4 Credit)

Max. Marks: 50

Duration: 32 Contact hours

Continuous Assessment: 10 marks

End Term Exam: 40 Marks

**Course Outcome:** On completion of the lab the student should be able to:

- Setup and monitor multistep synthesis in the laboratory.
- Monitor and analyze the progress of the reaction by TLC.
- Separate the mixture of compounds by column chromatography and their spectral analysis.
- Understand and develop the skills for extraction of natural products from plant or animal sources.

### SECTION A-INORGANIC CHEMISTRY

#### **A: Separation by Column Chromatography and Estimations:**

Experiment\_1: Separation of permanganate and dichromate ions on Alumina column and followed by estimation by *Permanganometry*

Experiment\_2: Separation of Cobalt (II) and Nickel (II) on an anion exchange column followed by estimation through EDTA back titrations.

#### **B: Spectrophotometry:**

Experiment\_3: Estimation of ferrous ions in a water sample with 1,10-Phenanthroline , spectrophotometrically

Experiment\_4: Analysis of Ferrous Iron in a Vitamin Pill

Experiment\_5: Estimation of inorganic Phosphorus in human serum, by Molybdenum blue method.

Experiment\_6: Determination of stoichiometry of Iron Thiocyanate complex using Job's Continuous variation method.

Experiment\_7: Determination of stoichiometry of Iron (II)—2,2-bipyridyl complex by Mole ratio method.

#### **C: Nano-chemistry:**

Experiment\_8: Synthesizing of silver nanoparticles (Ag NP) via chemical reduction: Understanding the Impact of Size on Silver's Optical Properties.

Experiment\_9: Synthesis of CdSeS nano-crystals exhibiting controllable photoluminescence.

### SECTION B-ORGANIC CHEMISTRY

#### **1 Multistep Organic Preparations (Synthesis)**

- (1) Synthesis of local anesthetics
- (2) Synthesis of analgesics.
- (3) Synthesis of sulpha drugs
- (4) Synthesis using microwaves: Alkylation of diethyl malonate with benzoyl chloride.
- (5) Skraup synthesis: Preparation of quinoline from aniline.
- (6) Beckmann rearrangement.
- (7) Aldol condensation: Dibenzal acetone from acetone and benzaldehyde.
- (8) Cannizarro's reaction of 4-Chlorobenzaldehyde.
- (9) Aromatic electrophilic substitutions in benzoic acid or aniline.

#### **2 Column Chromatography**

#### **3 Thin Layer Chromatography**

#### **4 Extraction of Natural Products**

- (a) Caffeine from Tea leaves
- (b) Lycopene and beta carotene from tomato

- (c) Citric acid from lemon juice
- (d) Keratin from human hair.

### **Spectral Analysis of synthesised/Isolated Compounds**

## **SECTION C-PHYSICAL CHEMISTRY**

### **A. Potentiometry**

1. Determination of strength and pK<sub>a</sub> value of weak acid by titration with an alkali using quinhydrone electrode.
2. Titration of Fe (II) vs. K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> and determination of standard redox potential of Fe<sup>2+</sup>/Fe<sup>3+</sup>.
3. Precipitation titration of KCl, KBr, KI and their mixture with AgNO<sub>3</sub>.

### **B. pH-metry**

1. Determination of pK<sub>a</sub> values of a tribasic acid by titration with an alkali.
2. Determination of H<sub>3</sub>PO<sub>4</sub> content in a given sample of Coca-Cola.
3. Determination of degree of hydrolysis of a given salt using pH-metry.

### **C. Spectrophotometry**

1. Determination of composition of a binary mixture of K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> and KMnO<sub>4</sub> or Cobalt (II) and Nickel (II) ions.
2. Spectrophotometric titration of Fe(II) vs. KMnO<sub>4</sub>.
3. To study the complexation reaction between Fe(III) & salicylic acid.
4. Recording Absorption spectra of a series of conjugated dyes-Application of the particle in one dimensional box. (Optional)

### ***Books Recommended:***

1. Vogel's quantitative analysis 6 Edn. Mendham, Denny; Pearson Education 2002
2. Modern Analytical Chemistry, David Harvey Mc Graw Hill. US
3. Analytical Chemistry. 7th edition, Gary D. Christian, Purnendu K. (Sandy) Dasgupta, Kevin A. Schug, Wiley
4. Experiments and Techniques in Organic Chemistry - D. Pasto, C. Johnson and M. Miller (Prentice-hall, 1992.)
5. Microscale and Macroscale Organic Experiments- K.L. Williamson (D.C. Heath and Co., 1989).
6. Advanced Practical Organic Chemistry, 2nd ed. - N.K. Vishnoi (Vikas, 1999).
7. Vogel's Textbook of Practical Organic Chemistry, 5th ed.- A.R. Tatchell (ELBS, • 1996)
8. Comprehensive Practical Organic Chemistry, V. K. Ahluwalia and Renu Aggarwal, (University Press-2000)
9. Practical Physical Chemistry, Findley, Kitchener, Longman, 1977.
10. Advanced Practical Physical Chemistry, Yadav, Goel Pub, 1994.
11. Experiments in Physical Chemistry, 5th ed., Schoemaker et al., MGH, 1989.

**Course No: CH21306DCE**  
**Title: Chromatographic Techniques (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 will acquire knowledge of:

- Classification and types of various chromatographic techniques and their principles.
- Thin Layer Chromatography, its stationary phase, mobile phase and principle of separation.
- Gas-Liquid chromatography, its principle, columns, stationary phase, resolution and instrumentation.
- High performance chromatography (HPLC), its importance and its versatility.

**Unit-I Chromatographic Techniques I (16 Contact hours)**

Introduction, Types and Classification, principles, differential migration, nature of partition forces, partition, Mobile phases, stationary phases, resolution, plate theory (concept), separation time, zone migration, column packing materials, development techniques, differential migration, partition coefficient, retention time and retention volume.

Thin layer chromatography: Theory, principle, adsorbents, preparation of plates, solvents, preparative TLC.

**Unit-II Chromatographic Techniques II (16 Contact hours)**

Gas-Liquid chromatography: Principle, columns and stationary phase, resolution and instrumentation.

HPLC: Theory, column efficiency, extra column and band broadening, temperature effects and diffusion. Chiral chromatography, chiral stationary phases. Applications of HPLC.

Ion exchange and size exclusion chromatography: Principle, mechanism of separation and applications.

***Books recommended***

1. Principles and Practice of Analytical Chemistry; 5<sup>th</sup> Edition; F. W. Fifield, D. Kealey; Blackwell Sciences Ltd.; 2000.
2. Modern Analytical Chemistry; David Harvey; McGraw-Hill; 2000.
3. Chromatographic Methods; 5<sup>th</sup> edn. ; A. Braithwaite and F. J. Smith; Kluwer Academic Publishers.
4. Fundamentals of Analytical Chemistry; 6<sup>th</sup> Indian Reprint; D. A. Skoog and D.M. West; Cenage Learning; 2012.
5. Thin layer Chromatography; E. Stahl and George Allen; Unwin Ltd. London.

**Course No: CH21307DCE**  
**Title: Bio-Physical Chemistry (02 Credits)**

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

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

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

- learn how to use the thermodynamic concepts and equations to explain the basis of different biological processes and quantify the different parameters associated with these processes.
- how basic thermodynamic equations can be used for estimation of thermodynamic parameters associated with biological processes
- how equilibrium thermodynamics can be used to understand the biological processes like protein folding, membrane potential and membrane transport, nerve conduction.

**Unit-I Biophysical Chemistry-I (16 Contact hours)**

Review of the basic concepts of Thermodynamics, Thermodynamics of living systems, Biochemists standard state, standard free energy changes in biochemical reactions, ATP as energy currency of cell, Principles of coupled reactions. Nernst equation, Standard potentials: Thermodynamic standard potentials, variation of potential with pH, the biological standard potential, converting standard potential to a biological standard value. Electron transfer in bioenergetics; Electron transfer reactions, oxidative phosphorylation. Biopolymers: Molecular forces and Chemical bonding in Bio-polymers, hydrophobic interactions, structure of proteins, protein folding and unfolding. Binding of Ligands and metal Ions to bio-macromolecules, one binding site per macromolecule, n equivalent binding sites per macromolecule, the Scatchard plot, binding of oxygen to myoglobin and haemoglobin.

**Unit-II Biophysical Chemistry-II (16 Contact hours)**

Biological membranes, Structure and functions of cell membrane, molecular motion across membranes, ion transport through cell membrane, Mechanism of Membrane Transport: Transport through cell membrane, active and passive transport systems. Irreversible thermodynamic treatment of membrane transport. Semipermeable membrane and Donnan membrane equilibrium, Donnan effect in Osmosis, its dependence on pH difference across the membrane. Membrane potential, Classical theory of membrane potentials; Nernst Equation, Nernst-Planck equation, permeability of membranes, Goldman-Hodgkin Katz model, Goldman equation, Nerve conduction; Action potential, factors affecting speed of action potential propagation, Nerve impulse and cardiovascular problems, Mechanism of vision. An introduction to bio-electroanalysis.

**Books recommended**

1. Physical Chemistry for the Biosciences, Raymond Chang, University Science Books, 2005.
2. Physical Chemistry for the Life Sciences, 2nd Edition, Peter Atkins, Julio de Paula, Oxford University Press 2015.
3. Biophysical Chemistry Part III: The behaviour of biological macromolecules, Charles R. Cantor and Paul R. Schimmel, W. H. Freeman and Company, New York, 2002.
4. Fundamentals of Biochemistry, D. Voet, J. G. Voet, C. W. Pralt, Wiley, 1999.
5. Lehninger Principles of Biochemistry, 7th Edition, Albert L. Lehninger, D. L. Nelson, N. M. Cox. W.H.Freeman& Co Ltd.

**Course No: CH21003GE**  
**Title: Bio-Organic 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:

- Recognize the importance of bio-organic chemistry and Pre-Biotic Chemistry.
- Understand formation and synthesis of carbohydrates and amino acids under pre-biotic conditions.
- Understand the mechanism of the function of enzymes, specificity and inhibition.

**Unit-I** **(16 Contact hours)**

**(a) Chemical Origins of Biology**

**Bio-organic chemistry:** Introduction, Basic consideration, Proximity effects in Organic Chemistry, Molecular rearrangements.

**Pre-Biotic Chemistry:** Role of HCN and HCHO in biosynthesis, Nucleophiles and Electrophiles in solution of HCN, Formation of Purines and Pyrimidines from HCN under prebiotic conditions. Carbohydrates from Aldol reaction with HCHO, Formation of Amino acids under prebiotic conditions.

**(b) Enzymes**

Introduction, Nomenclature and Classification of enzymes.

**Specificity of enzyme action:** Types of specificity, The active sites; The Fischer 'lock and key' hypothesis, The Koshland 'induced fit' hypothesis, Hypothesis involving strain or transition state stabilization.

**Enzyme Inhibition:** Introduction, Competitive inhibition, UnCompetitive inhibition, Non competitive, Allosteric inhibition.

**Unit-II** **(16 Contact hours)**

**(a) Coenzymes**

Introduction, Types of coenzymes, Involvement of coenzymes in enzyme catalysed reactions: Introduction, Nicotinamide Nucleotides (NAD<sup>+</sup> and NADP<sup>+</sup>), Flavin Nucleotides (FMN and FAD), Adenosine phosphate (ATP, ADP, AMP). Coenzyme A (CoA -SH ), Thiamine Phosphate, Biotin, Tetrahydrofolate, Coenzyme B<sub>12</sub> .

**(b) Biosynthesis of Natural Molecules**

Biosynthesis of Fatty Acids and Triglycerides, Biosynthetic Pathway of Terpenoids and Steroids, Inhibitors of Terpene biosynthesis, Biosynthesis of Flavonoids.

**Books recommended**

1. Introduction to Bioorganic Chemistry and chemical biology. D. V. Vranket and Gregory Weiss; Taylor and francis. 2013.
2. Bio-organicchemistry : Harman Dugas 3<sup>rd</sup> ed.Springer (2010) .
3. Bio-organic chemistry J.Rohr ,Springer (2000).
4. Enzymes 2<sup>nd</sup> ed. T. Palmer and P. Bonner (2008).
5. Biochemistry :DonaldVoet, Judith.G. Voet 2<sup>nd</sup>ed.Willey (1995)

**Course No.: CH21003OE**  
**Title: Medicinal Inorganic Chemistry**

**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 the sources of impurities and methods to determine the impurities in inorganic pharmaceuticals and know the mechanism of metal ion induced toxicity, metal ion promoted carcinogenesis and probable mechanism of action. Treatment of essential trace and ultra-trace element deficiencies and explain the method of preparation, assay, properties, medicinal uses of metal based complexes.
- Describe the properties, storage condition and application of radiopharmaceuticals

**Unit-I Medicinal Inorganic Chemistry-I (16 Contact hours)**

Metal toxicity and Homeostasis: sources of metal ion poisoning. Mechanism of metal ion induced toxicity(Pb, Cd, Hg, As, and Se) Toxicity of cyanide and nitrite ions. Metal ion promoted carcinogenesis and probable mechanism of action.

Metal based Therapeutic Compounds: Conditional stability constant, Stereochemistry, Lipophilicity. HSAB theory and Plasma mobilizing index(PMI). Therapeutic index of different chelating drugs in metal ion detoxification. Limitations and hazards of Chelation therapy

**Unit-II Medicinal Inorganic Chemistry-II (16 Contact hours)**

Treatment of essential trace and ultra-trace element deficiencies: Manganese, Iron, Copper, Cobalt, Zinc, Molybdenum, Silicon, Nitrogen and Phosphorus. Metal salts as anti-acids, antiseptics and diuretics.

Metal complexes as drugs: Vanadium based anti-diabetic drugs, Platinum based anticancer agents(cisplatin and its derivatives), non platinum based anticancer agents and Gold based anti-arthritic compounds and their mechanisms of action. Metal Complexes as anti-virals, anti-bacterials and anti-fungals;

Metal based Diagnostic agents: Technetium based radiopharmaceuticals. Gadolinium based MRI imaging agents. Radio protective chelating drugs.

***Books recommended:***

1. Bio inorganic Chemistry -An introduction; Ochai, Allyn and Bacon;1977.
2. Inorganic Aspects of Biological and Organic Chemistry; Hanzilik; Academic;1976.
3. The Inorganic Chemistry of Biological processes; 2nd edn.; Hughes ; Wiley;1973.
4. A Text book of Medicinal aspects of Bio inorganic Chemistry; Das; CBS;1990.
5. The Biological Chemistry of Elements; Frausto de Silva; Williams; Clarendon;1991.
6. Principles of Bio inorganic Chemistry; Lippard, Berg; Univ. Science Books; 1994.
7. Inorganic Chemistry in Biology; Wilkins C &Wilkins G; Oxford;1997.
8. Metal -Ions in Biochemistry; P. K. Bhattacharya; Narosa Publishing House;2005.
9. Bio-Inorganic Chemistry; Robert W. Hay; Ellis Horwood Ltd; 1984.
10. Concepts and Models in Bio-Inorganic Chemistry; Heinz-Bernhard Kraatz; Wiley; 2006.

**Course No: CH21401CR**  
**Title: Advanced Inorganic Chemistry (04 Credits)**

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

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

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

- To have an insight into structures of solid state inorganic materials like metal oxides, metal Hydroxides, MXenes, Pervoskites, MOFS, & Zeolites
- Conceptual understanding of structure- property relationship in functional inorganic materials by correlating structure with properties.
- Knowledge of standard synthesis methods of Inorganic Nanomaterials.
- Theoretical knowledge of Techniques & Methods for characterization & Analysis of Inorganic materials at Nano Level
- Understand how atomic arrangement & chemistry of inorganic material can give rise to functional properties and potential applications.

**Unit-I OrganoTransition metal Compounds: (16 Contact hours)**

**Sigma bonded OTMC:** Classification, Mechanistic pathways of kinetic instability, Routes of synthesis and reactions of  $\sigma$  OTMC, Decomposition Pathways: Choice, and mechanisms. Alpha, Beta hydrogen transfer reactions. Intramolecular elimination of alkane, Cyclometallation, Stability from bulky substituents, Agostic alkyls, Umpolung.

**Pi-Organometallic Compounds:** Comparison of  $\sigma$  and  $\pi$  OTMC, comparative bonding in Metal- alkene, alkyne, allyl, 1,3-butadiene and Cyclobutadiene Pi- systems.

Sandwich Compounds: Characteristics; Classification, Reactions and Structure and bonding of Ferrocene.

Compounds with Transition Metal to Carbon multiple bonds: Alkylidene (Schrock and Fischer) Synthesis; Structural characteristics; Nature of bonding. Reactions and their synthetic applications: Dotzreaction and Schrock's Catalyst.

**Unit-II Physico Chemical behaviour of OrganoTransition metal Compounds: (16 Contact hours)**

**A. Fluxional Organometallic Compounds:**

Characteristics; Rates of rearrangement and Techniques of study. NMR study of Fluxional behavior, Classification of Fluxional Organometallic Compounds. Mechanism of Fluxionality in compounds of  $\eta^1$  Cyclopentadienyls and  $\eta^3$ -allyls. Stereochemical non rigidity in case of coordination numbers- 4 & 5 (cis-trans, atomic inversion, Berry Pseudorotation).

**B. Catalytic processes involving OTMC:** mechanism of Hydrogenation, Hydroformylation, Oxidation and Isomerization of alkenes; Olefin metathesis. Monsanto acetic acid and Reppe reaction. Fischer-Tropsch Synthesis and Ziegler Natta polymerization of alkenes. Asymmetric, Photo redox catalysis and supported Organometallic Catalysis (brief idea)

**C. Synthetic Reactions involving Organometallics:**

Reactions of coordinated ligands, carbon monoxide and alkenes (Green, Mingo's rules). Role of organo-iron compounds as synthons, Activation of small molecules: prospectus and challenges. Selected reactivities for activation of Carbon monoxide, Carbon dioxide and Alkanes. Carbon-Carbon coupling reactions (Suzuki and Heck).

### Unit-III Inorganic Photochemistry; the basics

(16 Contact hours)

**A. Excited states:** Excitation: d-d transition, charge transfer & intra-ligand transitions and selection rules. Excited states; term symbols, splitting of terms in ligand field, Orgel diagram; electrostatic description of spin allowed d-d transitions & energy level diagrams depicting excited states.

Fate of excited states; energy dissipation by radiative and non-radiative processes. Jablonoski diagram.

Molar integrated absorption intensity, natural radiative lifetime & the calculation of life times.

**B. Kinetics:** Photochemical laws & quantum yield. Kinetics & quantum yield of photo-physical (radiative) and photo-chemical processes. Quantum Yields of a unimolecular and bimolecular photo-chemical reaction; Quenching and Stern-Volmer plots.

**C. Tools and Technique:** Chemical Actinometry. Time Resolved Spectroscopies: Time correlated Single photon counting technique Time Resolved Transient Absorption Spectroscopies: Flash Photolysis

### Unit-IV Electron Transfer in Excited Metal Complexes

(16 Contact hours)

**A. Marcus-Hush Model:** Energy transfer under conditions of weak and strong interaction. Excited state electron transfer. Conditions of the excited states to be useful as redox reactants. Photochemical electron transfer,  $[\text{Ru}(\text{bipy})_3]^{2+}$ ; Structure, excited state properties and photo chemistry as sensitizers

**B. Inorganic Photochemistry in practice:** Applications, Prospects and Challenges Solar energy storage and conversion. Photovoltaic Solar cells, Perovskite Solar cells, Dye sensitized and quantum dot sensitized solar cells. Metal oxide semiconductor based photo-splitting of water. Photochemical supra-molecular devices: devices for photo-induced energy or electron transfer, Devices for information processing, photo-chemically driven molecular machines Supramolecular photochemistry in natural systems: photosynthesis, bacterial photosynthesis and artificial photosynthesis

#### **Books Recommended:**

1. The Organometallic Chemistry of Transition Metals; 2<sup>nd</sup> and 4<sup>th</sup>edn; Robert. H . Crabtree; Wiley; 1994, 2004.
2. Fundamental Transition Metal Organometallic Chemistry; Luke hart; Brooks / Cole;1985.
3. Organometallic Chemistry; 2nd edn ; Mehrotra & Singh ; New age international2000
4. Principles and Applications of Organo Transition Metal Chemistry; Collman&
5. Finke; University Science Books;1994.
6. Principles of Organometallic Chemistry; 2nd edn.; P.Powel; Chapman & Hall;1998.
7. Metallo-Organic Chemistry; A.J.Pearson;Wiley.
8. Mechanisms of Inorganic and Organo metallic reactions; Twigg; Plenum press1983.
9. Reaction Mechanism of Inorganic and Organometallic systems; 2nd edn.; Robert .b. Jordan1998.
10. Inorganic Chemistry ; 4th edn.; Huheey ; E. Keiter& R. Keiter; Addison-Wesley;1983
11. Modern Inorganic Chemistry; William. A. Jolly; McGraw Hill;1985.
12. Inorganic Chemistry; 4\* edn; Huheey; Harper & Row; 1990.
13. Chemistry of Light; Suppan, Royal Society; 1994.
14. Photochemistry, Carol J. Wayne and Richard P. Wayne; Oxford University Press; 1996.
15. Fundamentals of Photochemistry; C Rohatgi, Mukhergi; Wiley Eastern.; 1992
16. Inorganic Photochemistry; J.ChemEdu.;Vol .60, No.10,1983.
17. Applications of Inorganic Photochemistry; J. Chem. Edu.; Vol.74, No 69. 1997.
18. Principles and applications of Photochemistry, Brian,Wardle, Wiley 2009



## Course No: CH21402CR

### Title: Advanced Organic Chemistry (4 Credits)

Max. Marks: 100

Duration: 64 Contact hours

Continuous Assessment: 20 marks

End Term Exam: 80 Marks

**Course Outcome:** On completion of the course the student should be able to:

- Understand various advanced methodologies used in the organic chemistry like asymmetric synthesis, disconnection approach and retrosynthesis.
- Understand the functions of various reagents and their applications in organic synthesis.
- Recognize the importance of the protection and deprotection of functional groups and their use in organic synthesis.

#### Unit I Methods in Organic Synthesis

(16 Contact hours)

**Asymmetric Synthesis:** Nature & asymmetry, Chiral pool approach, Chiral auxiliaries and auxiliary controlled stereoselection. Chiral reagents. Asymmetric formation of C-C bonds.: Asymmetric aldol, Heck and Baylis-Hillman reactions. Asymmetric hydrogenation and epoxidation of alkenes (Sharpless, Jacobsen and Shi reactions).

**Stereoselectivity:** Stereochemical control in six-membered rings, Stereoselectivity in bicyclic compounds.

**Diastereoselectivity:** Addition to carbonyl groups and stereoselective reactions of acyclic alkenes. Stereochemical reactions near a stereocenter.

Racemization & Resolution of enantiomers using chiral molecules.

**Chemoselectivity:** Selectivity in oxidation and reduction. Competing reactivity.

**Methods of multiple bond formations:** Carbon-Carbon and carbon heteroatom (N and O) bond formations with special emphasis on Metal catalysed bond formations (Ullmann, Buchwald-Hartwig, Sonogashira, Heck, Suzuki and Stille reactions).

#### Unit II Reagents in Organic Syntheses

(16 Contact hours)

Nature and applications of following reagents in organic syntheses: DABCO, DBU, DDO, Diglyme, DMAP, MCPBA, NCS, PCC, PDC, TBHP, TBAF, Lead Tetraacetate, Osmium Tetroxide, Aluminum isopropoxide, Prevost reagent, Woodward's Reagent, PdBaSO<sub>4</sub>, DDQ, DCC, SeO<sub>2</sub>, Ti(NO<sub>3</sub>)<sub>3</sub>, NaBH<sub>4</sub>, DIBAL, LAH, diisoamyborane, thexylborane, 9-BBN, NaIO<sub>4</sub>, Ceric ammonium nitrite, Palladium(II)hydroxalate, TEMPO, Ceric Ammonium nitrate(CAN), Fatesens reagent, MnO<sub>2</sub>. Na/EtOH and Na/liq.NH<sub>3</sub>.

#### UNIT-III PROTECTION AND INTERCONVERSION OF FUNCTIONAL GROUPS

(16 Contact hours)

Protection of functional groups: Principle of protection of functional groups and its significance. Protection of carbon-hydrogen bonds (in terminal alkynes and Carbon-hydrogen bond of aldehydes), carbon-carbon double bonds, alcoholic and Phenolic hydroxyl groups, amino groups, carbonyl and carboxyl groups.

Functional Group Interconversion (FGI) / Transformations: Significance of Functional Group Interconversion (FGI) / Transformations in Organic synthesis. Methods of transformation of different functional groups into one another. Chemoselectivity.

## Unit-IV Designing Organic Synthesis

(16 Contact hours)

**The disconnection approach:** Introduction to synthons, their types and equivalent reagents. Reversal of Polarity(umpolung). One group, two group and Reteroelectrocyclic disconnections. Reterosynthetic Analysis involving connections and rearrangements. Guidelines for good disconnections.

**One group disconnections:**Reterosynthetic analysis of alcohols, amines (aliphatic and aromatic), alkenes, carbonyl compounds, carboxylic acids and their derivatives using one group disconnections and FGIs. Use of acetylenes in the syntheses of above mentioned compounds.

**Two group disconnections:**Reterosynthetic analysis of 1, 2- difunctional compounds (1,2 – diols), 1,3- difunctional compounds (1,3-dioxygenated compounds,  $\alpha$ ,  $\beta$ -unsaturated carbonyl compounds, 3-amino alcohols and 3- amino ketones), 1,4- and 1,5-difunctional compounds.

**Multistep Synthesis:** Application of reterosynthetic analysis in designing /achieving syntheses of some complex molecules (for example Brufen, benziodarone, Juvabione, warfarin and brevicomin(Examples other than these may also be included).

### **Books Recommended**

1. Designing Organic Synthesis, S. Warren; Wiley; 2013.
2. Organic Synthesis- concept, methods and Starting Materials, J. Furhop and G. Penzlin; 1. Verlage VCH;1986.
2. Principles of Organic Synthesis2nd edn;. R. O. C. Norman; Chapman and Hall; 1978.
3. Advanced Organic Chemistry Part B, 5th edn.; F. A. Carey and R.J Sundberg ; Springer; 4. 2007.
5. Organic Chemistry, 10th edn;. T. W. G. Solomons and Craig B. Fryhle ; Wiley-2012.
6. Organic Chemistry; Clayden, Greeves, Warren and Wothers ; Oxford University Press-2012.
7. Organic Chemistry, David Klein; John-Wiley-2012.
8. Advanced Organic Chemistry: Reactions, Mechanism and Structure, 6th Ed., J. March,; Wiley; 2012.
9. Organic Synthesis- The disconnection Approach; Sturat Warren; Wiley; 2013.
10. Reagent Guide, Synthetic Organic Chemistry, & Materials Chemistry, 8th Edition.
11. Modern Methods of Organic Synthesis, Carruthers W. William Caruther and Iain Coldham, 4th edition.
12. A Guide to Reagents in Organic Synthesis., S Gupta, V Gupta, R.S Dhundal, 1st edition 2015
13. Transition Metal Reagents and Catalysts: Innovations in Organic Synthesis, by Jiro Tsuji, published: 17 July 2002.
14. Organic Synthesis, Jagdamba Singh, L.D.S Yadav, 1<sup>st</sup> Edition, 2006

**Course No: CH21403CR**  
**Title: Advanced 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:

- appreciate the importance of catalysts for green chemistry and development of sustainable chemical processes for industrial scale production of various chemicals/materials.
- learn as to how simple kinetic investigations and concepts acquired in the field of inorganic, organic and organometallic chemistry can be employed for the design of effective and stable catalysts for chemical transformations.
- get a knowhow of different types of catalysts, their mode of action, advantages and disadvantages, as well as their principal applications.
- understand the forces involved in the aggregation of molecules for the formation of soft matter relevant for life.
- get familiar with various soft materials formed by surfactants, polymers and block copolymers like hydrogels, liquid crystals and microemulsions
- understand the importance of the soft matter in environmental remediation, health, diagnosis, catalysis, development of smart materials, and fabrication of non-linear optical materials.

**Unit-I Catalysis-The Basics**

**(16 Contact hours)**

Overview of catalysis, homogeneous, heterogeneous and bio-catalysis, Replacing Stoichiometric Reactions with Catalytic Cycles, Potential functions of catalysts with examples; reaction initiation, intermediate/transition state stabilization (Sabatier's principle), reactant localization and reactant orientation, bond cleavage facilitation, electronic effect, reaction selectivity enhancement, energy and mass transfer facilitation effects of catalysts.

Kinetics of catalytic reactions. Catalyst deactivation, sintering, thermal degradation, Inhibition, poisoning.

Solvents as catalysts, solvation and its impact on reactant, product and transition state stabilization, impact of solvent on reaction rates, qualitative and semiquantitative predictions of the effect of solvents on reaction rates. Hydrophobic interactions, examples regarding facilitation of reaction kinetics and reaction selectivity via use of hydrophobic interactions.

**Unit-II Applied Catalysis**

**(16 Contact hours)**

**Catalysis by Metals:** Elementary reactions on metals, mechanism of metal catalyzed reactions, Trends over the periodic table, Metal Catalysts for specific organic transformations, Blowers-Masel equation for catalyst selection.

**Catalysis of Industrial processes:** Mechanistic and kinetic aspects of some selected industrial process; Synthesis of methanol, Fischer-Tropsch process, Synthesis of ammonia, Oxidation of ammonia, Photocatalytic breakdown of water. Catalysis and petroleum industry; catalytic reforming, catalytic cracking, cracking reactions and cracking catalysts.

**Industrial Bio-catalysis:** High-Fructose Corn Syrup, The Mitsubishi Rayon Acrylamide Process, The BMS Paclitaxel Process, The Tosoh/DSM Aspartame Process.

An introduction to catalysis in Energy-Related Environmental Technology.

### **Unit-III Introduction to Soft Matter, Amphiphiles, block copolymers and microemulsions (16 Contact hours)**

**Introduction to Soft Matter:** Constituents of soft matter, Intermolecular forces: van der Waals, electrostatic forces, covalent bond, hydrogen bond and hydrophobic interactions. viscoelastic response

**Amphiphiles:** General overview of self-assembly of amphiphiles. Introduction and applications of stimuli-Responsive surfactants: Biosurfactants, redox, photochromic, thermoreversible, pH-sensitive, cleavable and magnetic surfactants. Lipid bilayer, hydrophobicity: entropy driven interactions, self-assembly. Physics of membranes: elasticity, Helfrich energy. Plasma membrane: architecture, composition, Fluid mosaic model, membrane channels, active pumps, function.

**Block Copolymers:** Introduction: classification, micellization of diblock and triblock copolymers. Introduction to pH-, thermo- and Photo-responsive block copolymers. Applications.

**Microemulsions:** Emulsions and microemulsions, Physicochemistry of Microemulsions: Formation, Stability, and Droplet Clustering, Percolation Phenomenon in Microemulsions. Applications of microemulsions in cosmetics and detergency, pharmaceuticals, soil decontamination, enhanced oil recovery and biocatalysis.

### **Unit-IV Hydrogels, Langmuir Blodgett Films and Liquid crystals (16 Contact hours)**

**Hydrogels:** Introduction, Classification of hydrogels based on type of source, crosslinking and composition. Introduction to stimuli responsive hydrogels and their types. Rheological properties of hydrogels (steady-state, oscillatory and thixotropic behavior). Characterization of hydrogels. Applications of Hydrogels in adsorption, 3D printing, shape memory materials, drug release and other biomedical applications.

**Langmuir-Blodgett Films:** Introduction and general preparative techniques. LB Films of various compounds (hydrocarbon, liquid crystals compounds and polymers), Applications – nonlinear optical effects, conduction, photoconductivity and sensors.

**Liquid Crystals:** Mesomorphism, types of liquid crystals, molecular structural requirement of mesomorphism, properties of liquid crystals, Applications – Liquid crystal displays, thermography, optical imaging and ferroelectric liquid crystals.

#### ***Books Recommended***

1. Chemical Kinetics, K. J. Laidler, 3rd Edition, Pearson, 1987.
2. Chemical Kinetics and Reaction Dynamics, Paul L. Houston, Dover Publications, INC., Mineola, New York, 2001.
3. Chemical Kinetics and Dynamics, J. I. Steinfeld, J. S. Francisco, W.L. Hase, Prentice Hall, 1989
4. Chemical Kinetics and Catalysis, R.I. Masel, Wiley, 2001
5. Chemical Kinetics: From Molecular Structure to Chemical Reactivity, Luis G Arnaut, Sebastiao Jose Formosinho, Hugh Burrows, Elsevier, 2007.
6. M. J. Rosen, J. T. Kunjappu, "Surfactants and Interfacial Phenomena", John Wiley & Sons, New York, 4<sup>th</sup> Edition, 2012.
7. D. Fennell Evans, H. Wennerstrom, "The Colloidal Domain where physics, chemistry, biology and technology meet" VCH, New York, 1994.
8. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
9. I. W. Hamley, The Physics of Block Copolymers (Oxford University Press, Oxford, 1998).
10. N. Hadjiichristidis, S. Pispas and G. A. Floudas Block Copolymers (Wiley, New York, 2003).

**Course No: CH21404CR**  
**Title: Project Seminar and Dissertation (02 Credits)**

**Max. Marks:50**

**Course Outcome:** On completion of the lab project the students will be required to prepare a dissertation based on their lab project work. The students will also be required to deliver a PowerPoint presentation for evaluation.

**Course No: CH21405DCE**  
**Title: Lab Project in Chemistry (04 Credits)**

**Max. Marks:**100

**Duration:** 3 lab session of one hour each per day

**Course Outcome:** On completion of the lab project the student should be able to:

- Design and setup various kinds of organic reactions in the laboratory.
- Monitor and analyze the progress of the reaction, and take appropriate measures to ensure its successful completion.
- Use catalysts, reagents and substrates keeping in mind the green chemistry practices.
- Separate the mixture of compounds by column chromatography and their analyses.
- Understand and develop the skills for extraction of compounds from plants and evaluation of their biological profile.

**Course No: CH21406DCE**  
**Title: Inorganic Materials (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

- To have an insight into structures of solid state inorganic materials like metal oxides, metal Hydroxides, MXenes, Pervoskites, MOFS, & Zeolites
- Conceptual understanding of structure- property relationship in functional inorganic materials by correlating structure with properties.
- Knowledge of standard synthesis methods of Inorganic Nanomaterials.
- Theoretical knowledge of Techniques & Methods for characterization & Analysis of Inorganic materials at Nano Level
- Understand how atomic arrangement & chemistry of inorganic material can give rise to functional properties and potential applications.

**Unit-I Transition Metal Based Functional Materials (16 Contact hours)**

**History**, development and importance of functional inorganic materials. Transition metal-based materials: Synthetic routes, structure and applications of Metal oxides, Metal hydroxides.

**Synthetic routes**, structure and applications of MXenes and Pervosikites. MXenes - Li and Na ion batteries, Super capacitors and Optoelectronic devices. Pervosikites - Solar cell applications

**Zeolite Molecular Sieves:** Structure, Chemistry, and applications

**Metal Organic Frameworks (MOFs):** Synthetic routes, structure and applications of Metal Organic Frameworks (MOFs):

Characterization methods, Isorecticular series. Application in gas storage and separation.

MOF thin films for separation and catalysis. Medical applications of MOFs

**Unit-II: Inorganic Nano Materials (16 Contact hours)**

Definition, development and importance of Nano materials

**Metal and metal-oxide Nanoparticles:** Synthetic routes: synthesis by Chemical methods: reduction, Solvothermal/hydrothermal route, electrospinning. Micro-emulsion method, templating method, combustion method, microwave synthesis, gas phase method, and conventional Sol-Gel method.

**Structure and properties.** Band structure, Band gaps, Quantum Dots. Nanosize effects- Quantum confinement effect, Size dependent physical phenomenon in nano materials. Optical and mechanical properties of nano materials.

Electrical properties, electron transfer and charge transport

**Analysis methods** (elementary idea): Powder X-ray diffraction, Electron Microscopy (SEM and TEM), Scanning probe microscopy (AFM, STM)

**Applications** in the fields of solar cells, light-emitting diodes, transistors, optoelectronic packaging, photo-catalysis, sensors and coatings

***Books/ Research Papers Recommended:***

1. G. Cao, Nanostructures and Nanomaterials: Synthesis, properties and applications, Imperial College Press, 2004.
2. C. N. R. Rao, A. Muller, A. K. Cheetham, The chemistry of nanomaterials: Synthesis, properties and applications, Wiley (2004).
3. Hornyak, Dutta, Tibbals and Rao, Introduction to Nanoscience and Nanotechnology, New York, CRC press, 2008
4. J. Goldstein, D. E. Newbury, D.C. Joy, and C.E. Lym, "Scanning Electron Microscopy and X-ray Microanalysis", 2003.
5. D. Williams and B. Carter, "Transmission Electron Microscopy - A Textbook for Materials Science", Plenum Press, New York, 2nd Edition, 2009
6. Solid State chemistry, AR West
7. Y. Leng, Materials Characterization-Introduction to microscopic and spectroscopic methods. Second Edn. Wiley-VCH



**Course No: CH21407DCE**  
**Title: Supramolecular Chemistry (02 Credits)**

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

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

**Course Outcome:** The course focus on understanding the nature of intermolecular interactions, responsible for aggregation and consequent material properties and applications. Chemistry behind working and fabrication of molecular devices and sensors is dealt with to provide students an apprehension to understand design, working and fabrication of applied materials.

**Unit-I Supramolecular Chemistry (16 Contact hours)**

**A. Acid-Base Theories-**

Overview of Acid-Base theories. Hard Soft Acid Base (HSAB) Concept– Introduction, Classification, Symbiosis, PearsonPauling Paradox.

Utility of HSAB Concept in Drug Design, Quantitative Analyses of Metal Cations and Prediction of Direction of Inorganic Reactions.

**B. Supramolecular Chemistry**

Definition and Development of Supramolecular Chemistry. History and Genesis of the Nobel Prizes Awarded in the Area. Types and Nature of Supramolecular/Non-Covalent Interactions: Hydrogen Bonding,  $\pi$ - $\pi$  Interactions, Halogen Bonding, van der Waal Interactions. Quantification of non-covalent interactions through computational method: Electrostatic Potential Maps, de-di and fingerprint Plots.

**Unit –II Crystal Engineering (16 Contact hours)**

Definition and Development of Crystal Engineering.

Hydrogen bonding: Definition, Nature and Importance. Classification of Hydrogen Interactions.

Identification of Weak, Moderate and Strong Hydrogen Bonds.

Crystal Engineering of organic molecules: Co-crystals and Molecular Salts. Pharmaceutical Co-crystals. Polymorphism. Crystal Engineering of inorganic molecules: Coordination Complexes and Metal Organic Frameworks (MOFs)

**Transformation of Molecules into Devices**

Supramolecular Sensors and Devices-Thermochromism, Solvatochromism and Photophysics. Charge Transfer Complexes. Theory of  $\pi$ - $\pi$  Stacking. Degree of Charge Transfer. Organic Conductors and Semiconductors. Organic Light Emitting Diodes (OLEDs) and Transistors. Organic Lasers (Elementary Idea)

### ***Books/Research Articles Recommended***

1. Supramolecular Chemistry. Jonathan W. Steed and Jerry L. Atwood. Wiley 2nd Edn.
2. Supramolecular Chemistry-Fundamentals and Applications. A. Katsuhiko and K. Toyoki. Springer.
3. Crystal Engineering. G. R. Desiraju, J. J. Vittal and A. Ramanan. World Scientific, 1st Edn.
4. Organic Crystal Engineering: Frontiers in Crystal Engineering. E. R. T. Tiekink, J. Vittal and M. Zaworotko. Wiley, 2010.
5. Frontiers in Crystal Engineering. Edward R. T. Tiekink (Editor), Jagadese Vittal (Editor). Wiley, 2005.
6. An Introduction to Supramolecular Chemistry. Asim K. Das, Mahua Das, CBS Publishers and Distributors Pvt Ltd. 2005.
7. Introduction: Supramolecular Chemistry. Huang, F.; Anslyn, E. V. Chem. Rev. 2015, 115, 6999-77000.
8. Supramolecular materials. Amabilino, D. B.; Smith, D. K.; Steed, J. W. Chem. Soc. Rev., 2017, 46, 2404-2420.
9. A Bond by Other Name. Desiraju, G. R. Angew. Chem. Int. Ed. 2011, 50, 52-59.
10. The Weak Hydrogen Bond: In Structural Chemistry and Biology. Desiraju, G.; Steiner, T. Oxford, IUCr Monograph on Crystallography.
11. Application of the Principle of Hard and Soft Acids and Bases to Organic Chemistry. Pearson, R. G.; Songstad, J. J. Am. Chem. Soc. 1967, 89, 1827-1836.

**Course No: CH21408DCE**  
**Title: Medicinal 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:

- Understand types of drugs and drug discovery process.
- Correlate structure with biological activity and quantitative analysis of structure activity relationships of drug molecules.
- Comprehend the mechanism of the function of drugs used as antipyretic, analgesic, antibiotic, psychoactive, cardiovascular and antiviral medicines.

**Unit-I Medicinal Chemistry-I (16 Contact hours)**

**Drug Design:** Classification and sources of drugs, concept of lead compounds and lead modification. Analogues, prodrugs, factors governing drug design.

**Structure activity relationship (SAR):** Isosterism, bioisosterism, changing the size and shape, changing the number of methylene groups in chain, changing the degree of unsaturation. Effect of introduction of methyl groups, halogens, hydroxyl, carbonyl, thiols, sulphide groups and introduction/removal of ring systems on pharmacological activity.

**Quantitative structure activity relationships (QSAR):** Theories of drug activity, Clark's occupancy theory, the rate theory, two state theory. Lipophilic constant, Hammett constant, steric parameters and Hansch analysis.

**Antipyretics Analgesics:** Paracetamol, Acetaminophen, Aspirin, Acetanilide, Salicylamide, Benzydol, Phenazone, Dipyrone, Mefenamic Acid,

Synthesis of Diuretics, Anti-inflammatory, Muscle relaxants, Antihistaminic drugs, Uricosurics (Anti-gout-Agents), anti-coagulants.

Synthesis of naturally occurring bioactive compounds (Vitamin A, C and D), Prostaglandins.

**Unit-II Medicinal Chemistry-II (16 Contact hours)**

**Antibiotics:** Penicillins-classification and structures. Synthesis of Penicillins, V, G, chloramphenicol and ciprofloxacin. Tetracyclins.

**Psychoactive Drugs:** Introduction, CNS depressants, CNS stimulants, sedatives and hypnotics, barbiturates. Synthesis of diazepam, phenytoin and glutethimide.

**Cardiovascular Drugs:** Introduction, cardiovascular diseases, synthesis of Amyl nitrate, sorbitrate, quinidine, verapamil, methyl dopa and atenolol.

**Antiviral Drugs:** Chemistry of Viruses, Mechanism of action, Synthesis of indinavir, Noval Corona Virus; variants and the vaccinations.

**Books Recommended:**

1. Introduction to Medicinal Chemistry, Alex Gringauz (Wiley- VCH-1997).
2. Medicinal Chemistry- An Introduction, Gareth Thomas (Wiley-2000). 3rd Edition.
3. Medicinal Chemistry, Ashutosh Kar. (Wiley Eastern-1993).
4. Biochemistry, Biotechnology and Clinical Chemistry of Enzymes. Trevor Palmer (EWP)
5. Organic Chemistry by I. L. Finar Vol. II ( ELBS Longman)
6. Lehninger's Principles of Bio-chemistry, D.L. Nelson. M.Cox Worth publications, 2000.
7. Introduction to nucleic acids and related natural products Ulbight (Oldborn Press )
8. Chemistry of Natural Products. S.V. Bhat, B.A. Nagasampagi, M. Siva Kumar. Narosa

**Course No: CH21409DCE**  
**Title: Chemistry of Natural Products (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:

- Understand the role and importance of natural products in medicine and drug discovery.
- Recognise the chemistry and spectroscopic methods involved in structure determination and synthesis of different classes of natural products *viz* terpenoids, steroids, alkaloids and flavonoids.

**Unit-I: Terpenoids and Steroids (16 Contact hours)**

**Terpenoids:** Introduction and classification. Chemistry of Citral/Geraniol,  $\alpha$ -Terpeniol, Camphor, Zingiberene and Vitamin A. Biogenesis of terpenoids.

**Steroids:** Introduction and classification. Chemistry of cholesterol, Progesterone, Oestrone, Cortisone and Androsterone. Biogenesis of cholesterol.

**Unit-II ALKALOIDS AND FLAVONOIDS. (16 Contact hours)**

**Alkaloids:** Introduction, qualitative tests and general methods of isolation. Structural elucidation synthesis and biogenesis of Reserpine and Morphine.

**Flavonoids:** Introduction, qualitative tests and general methods of isolation. Structure and synthesis of Apigenin, Quercetin, Genistein and Anthocyanidin. Antioxidant properties of Flavonoids.

**Books Recommended:**

1. Chemistry of Natural Products; S. V. Bhat, B. A. Nagasampagin. (Narosa 2005).
2. Organic Chemistry, 5th Ed. Vol.2,1. L. Finar (Addison Wisley Longman-2000).
3. Chemistry of Natural Products, N.R. Krishnaswamy (University Press-1999).
4. Flavonoids; Oyvind M. Andersen and Kenneth R. Markhan. (Taylor & Francis -2006)
5. The Flavonoids, Jeffrey B. Harborne, Tom J. Mabry, Helga Mabry, Academic Press 1975

## Course No: CH21410DCE

### Title: Computational and Advanced Quantum Chemistry (02 Credits)

Max. Marks: 50

Continuous Assessment: 10 marks

Duration: 32 Contact hours

End Term Exam: 40 Marks

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

- appreciate the potential of numerical methods to solve the complex mathematical equations like simultaneous equations, integrals, differentials, determinants, eigen value problems etc.
- have in depth understanding of use of MS Excel as easily available tool to solve above equations numerically.
- get knowhow of the Hartree Fock and Density functional theories to evaluate the energy and other properties of multielectron systems using slater and gaussian wave functions.
- get acclimatized with the gaussian software for running HF or DTF methods for evaluating energy, getting optimized geometry, predict NMR, UV-Vis frequency etc.

#### Unit-I Numerical Methods

(16 Contact hours)

Basic theory, discussion of algorithms and errors for following numerical methods:

##### (a) Numerical solution of equations

**Solution of Equations:** Bisection, Newton-Raphson method for solving polynomial and transcendental equations. Convergence. Errors and ill-conditioning

**Linear Simultaneous equations:** Gaussian elimination and Gauss-Siedel method. Errors and ill-conditioning.

**Eigen values and Matrix Diagonalization:** Eigen value problem, diagonalization of a matrix, Jacobi and Householder methods.

##### (b) Numerical differentiation

**Numerical differentiation:** Solutions of simple differential equations by Taylor series and Runge-Kutta methods.

##### (c) Numerical Integration

**Numerical integration:** Newton-Cotes formulae, Romberg integration, errors in integration formulae.

##### (d) Interpolation and Curve Fitting

Lagrange's interpolation method, Newton's divided differences, Cubic spline, piece wise interpolation. Least squares approximation, linear and quadratic.

#### Unit-II Advanced Quantum Chemistry

(16 Contact hours)

##### *ab initio* Calculations of Electronic Structure

##### a) Hartree-Fock Self Consistent field method:

Hartree-Fock method: Coulomb and exchange operators and integrals, Roothaan equations: the Fock matrix elements, Koopman's theorem. Self Consistent Field procedure. Slater-type orbitals (STOs), Gaussian type orbitals (GTOs), Basis Sets: minimal basis set, split-valence basis set, Polarization basis sets. Model SCF calculations on  $H_2/HeH^+$ .

**b) Beyond Hartree-Fock method:**

**Electron correlation:** configuration state functions, configuration interaction (CI) and its calculations.

**Density Functional Theory (DFT):** Introduction, electron probability density, Hohenberg-Kohn theorems and Kohn-Sham formulation of DFT.

**c) Use of Gaussian quantum mechanical package for:**

1. A single point energy calculation: HCHO /CH<sub>3</sub>CHO, HCHO MOs.
2. Geometry Optimization: Input and Output for ethene, fluoroethene, propene conformers. Basis set effect on geometrical parameters on these molecules.
3. NMR properties of ethane, ethene and ethyne.
4. Frequency Calculations: Input, Formaldehyde frequencies, Normal modes, zero point energy, thermodynamic properties, polarizability, hyperpolarizability.
5. Selecting an appropriate theoretical method:
  - a) Electron correlation and post SCF methods, limitations of Hartree-Fock theory: HF bond energy, Optimization of O<sub>3</sub>.
  - b) Density Functional Theory: CO<sub>2</sub> structure and atomization energy.

***Books Recommended***

1. Data Reduction & Error Analysis, Bevington & Robinson, (McGraw-Hill, 2003)
2. Numerical Methods for Scientists and Engineers, H. M. Antie, (TMH, ).
3. Mathematical Methods for Scientists and Engineers, D.A. McQuarrie, Viva Books, 1st Ed., 2009.
4. Quantum Chemistry, Ira. N. Levine, (Prentice Hall, 2009).
5. Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedmann, (Oxford, 2008).
6. Quantum Chemistry and spectroscopy, Engel & Reid, Pearson (2007)
7. Modern Quantum Chemistry - Introduction to Advanced electronic structure theory - A. Szabo & N. S. Ostlund, (Macmillan, 1982, Dover 1996).
8. GAUSSIAN Manual, Gaussian Inc
9. Exploring chemistry with electronic structure methods, Foresman J.B., Frisch A., Gaussian Inc

**Course No: CH21411DCE**  
**Title: Applied Electrochemistry (02 Credits)**

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

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

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

- appreciate the potential utility of electrochemical methods for sensing and detoxification of pollutants, solar energy harvesting, energy generation and storage
- learn about the basic principles, design and applications of photoelectrochemical cells.
- learn about how to use electrochemical methods for detoxification of pollutants especially water contaminants
- learn about the basics of fuel cells and batteries, the design, operation and challenges associated with the different types of such systems in energy applications.

**Unit-I Applied Electrochemistry-I (16 Contact hours)**

**Photo- and Environmental Electrochemistry**

**Photo-electrochemistry:** Semiconductor electrodes, Band bending across Semiconductor/electrolyte solution interface, photo-electrochemistry across semiconductor/electrolyte interfaces, p-type photocathode, n-type-photoanode, surface effects in photo-electrochemistry, Photogalvanic and Photovoltaic Cells, The Efficiency of Solar Energy Conversion in Photoelectrochemical Cells, Liquid-Junction Solar Cells: Principles of Operation and Energetics of Conversion.

Photoelectrochemical splitting of water, Photoelectrochemical reduction of CO<sub>2</sub>, Production of solar fuels.

**Environmental Electrochemistry:** Positive Features of Electrochemical Remediation. Direct Electrolysis of Pollutants. Indirect Electrolysis of Pollutants. Electroremediation of Soils.

Water Disinfection: Background and Principles. Electrochemical Disinfection of Water, electro dialysis, Photoelectrochemical Disinfection of Air and Water.

**Unit-II Applied Electrochemistry-II (16 Contact hours)**

**Electrochemistry for Energy Conversion and Energy Storage**

**Fuel Cell:** Basic principles, advantages and limitations, fuel cell performance.

**Fuel Cell Thermodynamics:** Open circuit voltage, efficiency and efficiency limits, efficiency and fuel cell voltage. Operational fuel cell voltage; fuel cell irreversibilities, causes of voltage drop.

**Types of fuel Cells:** Alkaline, Phosphoric acid, Polymer Electrolyte membrane and direct MeOH fuel cell, biofuel cells.

**Energy storage devices:** Desirable characteristics of energy storage devices, Discharge plot, Ragone plot.

**Batteries:** How batteries work, Battery characteristics, Battery specification, Battery components. Primary and secondary batteries, Measures of battery performance. Classical batteries (Lead Acid, Nickel-Cadmium, Zinc-Manganese dioxide). Modern batteries (Zinc-Air, Nickel-Metal Hydride, Lithium Ion Batteries).

**Books Recommended**

1. Electrochemical Methods Fundamentals and Applications, 2<sup>nd</sup> Edition, Allen J. Bard, Larry R. Faulkner, John Wiley and Sons, INC.
2. Physical Electrochemistry: Fundamentals, Techniques, and Applications, 2<sup>nd</sup> Edition, Eliezer Gileadi and Noam Eliaz, 2018, Wiley-VCH.

3. Electrochemistry, 2nd Edition, Carl H. Hamann, Andrew Hammett, Wolf Vielstich, Wiley-VCH.
4. Modern Electrochemistry 2B, 2nd Edition, J. O`M. Bockris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.
5. Fuel Cell Fundamentals, 3<sup>rd</sup> Edition, Ryan O'Hayre, Suk-Won Cha, Whitney Colella, Fritz B. Prinz, John Wiley & Sons.
6. Understanding Batteries, Ronald Dell, David Anthony James Rand, Royal Society of Chemistry, 2001.
7. Industrial Electrochemistry, 2<sup>nd</sup> Edition, D. Pletcher, F. C. Walsh, London, GB. Chapman & Hall.
8. Environmental Electrochemistry, 1st Edition, Krishnan Rajeshwar, Jorge Ibanez, Academic Press, 1997.



**Course No: CH21004GE**

**Title: Synthetic Polymers and their Applications (02 Credits)**

**Max. Marks: 50**

**Continuous Assessment: 10 marks**

**Duration: 32 Contact hours**

**End Term Exam: 40 Marks**

**Course outcomes:** On completion of the course, the students will acquire knowledge of:

- Basic concepts about polymers.
- Different types of mechanism involved in polymerization processes.
- Chemistry of commercially important polymers.
- Chemistry of natural rubber and polysaccharides.

**Unit-I**

**(08 Contact hours)**

Introduction, Definition, Classification based on source, Structure, Synthesis and Forces of attraction. Thermosetting and Thermosensitive plastics, Types of Monomers, Homopolymers and Copolymers.

**Unit-II**

**(08 Contact hours)**

Polymerisation processes, Addition polymerization, Free radical, Cationic, Anionic mechanism of addition polymerization Initiators, Inhibitors and Propagators. Stereochemical control of polymerization- Zeiglar Natta catalysts, Poly condensation; Polymerisation.

**Unit-III**

**(08 Contact hours)**

Commercially important polymers: Polyesters, Polycarbonates, Polyamides, Polyurethanes, Poly sulphides, Resins: Phenol-formaldehyde and Melamine-formaldehyde resins. Conducting Organic Polymer (elementary idea), Biodegradable polymers

**Unit-IV**

**(08 Contact hours)**

**Natural polymers:** Rubber, Vulcanization,

**Polysaccharides:** Cellulose, Amylopectin and Starch, Proteins; Wool, Silk and Collagen; Regenerated properties.

**Books Recommended**

1. Organic chemists: Francis . A. Carey, Robert M. Giuliano. 8<sup>th</sup> ed. Tata Mc Graw Hill. 2010
2. Polymer chemistry- An introduction. Mallolin. P. Steven, 2<sup>nd</sup> ed. Oxford University. 1998
3. Organic chemistry: L. G. Wade, Tr. Maya Shankar Singh. 6<sup>th</sup> ed., 2005, Pearson.
4. Introduction to polymers: 2<sup>nd</sup> ed. R.J. Young and P.A. Lovell. Chapman and Hill
5. Organic chemistry: David Klein; Willey 2012 .

**Course No: CH21005GE**  
**Title: Novel Materials (02 Credits)**

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

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

**Unit-I Block Co-Polymers, Langmuir Blodgett Films and Organic Solids**  
**(16 Contact hours)**

**Block Copolymers:** Introduction: classification, micellization of di block and triblock copolymers. Introduction to pH-, thermo- and Photo-responsive block copolymers. Linear-dendrimer block copolymers: introduction, structural peculiarities of their aggregates, potential applications.

**Langmuir-Blodgett Films:** Introduction and general preparative techniques. LB Films of various compounds (hydrocarbon, liquid crystals compounds and polymers), Applications—nonlinear optical effects, conduction, photo conductivity and sensors.

**Organic solids and fullerenes:** Organics conductors, organic super conductors. Fullerenes—History, bonding, properties, doped fullerenes, fullerenes as superconductors. Carbon nanotubes: Types, Properties and Applications.

**Unit-II Optical and Nano-materials:** **(16 Contact hours)**

Luminescence and phosphors. Lasers - general principle of lasing action, Ruby laser, semi-conducting lasers and quantum cascade lasers.

Nonlinear optical effects, second and third order harmonic generation, nonlinear optical materials.

**Liquid Crystals:** Mesomorphism, types of liquid crystals, molecular structural requirement of mesomorphism, properties of liquid crystals, Applications—Liquid crystal displays, thermography, optical imaging and ferroelectric liquid crystals.

**Nanomaterials:** Introduction with examples and applications of nanoparticles, nanofibers (nanowires, nanotubes and nanorods) and nanoplates.

**Composites:** Polymer-nano-object blends, Metal-Matrix composites, self-repairing composites and Nano fluids for Thermal transport.

**Books Recommended**

1. Solid State Chemistry and its Applications, West, Wiley, 2014.
2. The Physical Chemistry of Solids, Borg, Biens, Academic press, 1992.
3. Solid State Physics, N. W. Ashcroft and N. D. Mermin, Saunders college, 2001
4. Principles of Solid State, H. V. Keer, Wiley Eastern; 2008.
5. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
6. The Physics and Chemistry of materials, J.I. Gersten, F.W. Smith, John Wiley and sons, Inc. 2001.
7. New directions in solid state chemistry, C.N.R. Rao and J. Gopalakrishnan, Cambridge University Press, 2nd ed.
8. Nanotechnology, An Introduction, J. J. Ramsden, Elsevier, 1st Edition, 2011.
9. Essentials of Nanotechnology, J. J. Ramsden, J. Ramsden and Ventus Publishing ApS, 2009.

**Course No: CH21004OE**  
**Title: Food 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 students will acquire knowledge of chemistry involved in:

- Different components of food.
- Different Pigments in animal and plant tissues.
- Food colorants & flavorings.
- Food Preservation & food additives.

**Unit-I** **(16 Contact hours)**

**(a) Food Components**

Chemistry of different components of food: Composition and functions of Sugars, Polysaccharides, Lipids, Proteins, Vitamins and Minerals.

**(b) The Chemistry of Food Colours and flavours**

Introduction. Pigments in animal and plant tissues: Chlorophyll, Carotenoids, Anthocyanins and other Phenols. Natural and artificial food colorants. Definition of flavor. Classification of food flavors. Chemical components responsible for the following: Sweetness, Saltiness, Sourness, Bitterness, Astringency, Pungency, Meatiness and Fruitiness. Synthetic flavouring.

**Unit-II** **(16 Contact hours)**

**(a) The Chemistry of Food Preservatives:**

Introduction. Basis of Food Preservation. Food additives: Sodium Chloride, Nitrites, Smoke, SO<sub>2</sub>, Benzoates and other Organic acids.

**(b) The Undesirables in Food Stuff**

Autooxidation and antioxidants. Modified atmosphere and vacuum packaging. Toxins of plant foods. Toxins of animal foods. Toxic agriculture residue Toxic metal residue. Toxins generated during heating and packaging of food. Environmental pollutants of food stuff.

**Books Recommended**

1. Food Chemistry; Owen R. Fennema; 3<sup>rd</sup> Ed.; Marcel Dekker, Inc. NY; 2005.
2. Food: The Chemistry of its components; T.P. Coultate; 3<sup>rd</sup> Ed.; RSC Paperbacks; 1996.
3. Food Flavours; Biology and Chemistry; Carolyn Fisher and Thomas R Scott; RSC Paperbacks; 1997.
4. Food Preservatives; H.J. Russell and G. W. Gould; 2<sup>nd</sup> ed.; Springer International Edition; 2005.