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

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

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

- Know about the thermodynamic stability of metalcomplexes 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 complexesand the nature of interaction in other π-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^nconfiguration and lability,Stability of uncommon oxidation states.Metal Chelates: Characteristics, Chelate effect and the factors affecting stability of metalchelates. Ligand preorganization, Macrocyclic effect Complexes of Crown ethers andCryptands, Tertiary phosphine as ligand.Determination of formation constants by pH- metry and spectrophotometry.Structural (ionic radii) and thermodynamic (hydration and lattice energies) effects of crystalfield 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 favorof 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 pibonding.(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 anddioxygen 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 protectivechelating 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, β-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 Imagining (MRI). lanthanide Single molecule magnets

Books Recommended:

1. Lanthanide and Actinide Chemistry; Simon Cotton; 2nd Revised Edn.; John Wiley & Sons: West Sussex, England; 2006.
2. Inorganic Chemistry; Weller, Overton, Rourke, Armstrong; 6thEdn.; Oxford University Press; 2017 Reprint
3. Inorganic Chemistry; G. Wulfsberg; Viva Books Private Limited; 2005 Reprint
4. Chemistry of the Elements; 2ndEdn; N. N. Greenwood, A. Earnshaw; Elsevier; 2014 Reprint
5. Inorganic Chemistry; 3rdEdn; D. F. Shriver; P. W. Atkins; Oxford; 1999.
6. Advanced Inorganic Chemistry; Vol-1, 34th Reprint 2013; Krishna Educational Publishers
7. Concise Inorganic Chemistry; J. D. Lee; 5thEdn.; 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 **Duration: 64 Contact hours**
Continuous Assessment: 20 marks **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 andsp 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 π-electron numbers other than six (2,4,8,10 and more than ten π-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, alkylidine 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, 6th Ed., Smith, M.B. (Wiley-2014)
2. Organic Chemistry 8th Ed. - F. A. Carey and Robert M. Giuliano (McGraw Hill-2012).
3. Reaction Mechanism in Organic Chemistry RevisedEd., S.M. Mukherjee and S.P. Singh. (Macmillan- 2017).
4. Organic Chemistry - 2nd Ed., J. Hornback. (Brooks/Cole- 2006).
5. Organic Chemistry, 5th Ed., John McMurry. (Brooks/Cole-2000).
6. Advanced Organic Chemistry, 5th Ed., F.A Carey & R.J Sundberg (Springer-2007).
7. Organic Chemistry, 2nd Ed., Jonathan Clayden (OUP-2016).
8. Organic Chemistry, 11th Ed., Solomons, T.W.G., (Wiley-2015).
9. Organic chemistry, Morrison, Boyd and Bhattacharya. 7th Ed. Pearson-2013.
10. Stereochemistry of Organic Compounds 2nd Ed., D. Nasipuri. (New Age Inter.- 2008)
11. Stereochemistry of Carbon Compounds - E.L.Eliel. (TMH -2007)
12. Stereochemistry of Organic Compounds 7th Ed. - P.S. Kalsi. (New Age Inter.- 2012).

Course No: CH21103CR
Title: Physical Chemistry (04 Credits)

Max. Marks: 100 **Duration: 64 Contact hours**
Continuous Assessment: 20 marks **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), Hammet 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. 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. 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 **Duration: 32 Contact hours**
Continuous Assessment: 10 marks **End Term Exam: 40 Marks**

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

Atmosphere: Vertical profile of theatmosphere; troposphere creactivity patterns; stratospheric chemistry (Chapman mechanism and ozonedepletion).

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 conceptand Pourbiaxdiagram and oxygen sag curve).
Chemistry of watert reatment: Chlorination, Ozonationand 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; 2nd 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; WileyEastern; 1995.
5. Environmental pollution Analysis; S.M.Khopkar;WileyEastern.
6. Environmental Chemistry; S.E.Manahan (6th /7th /8th/9thEdns); LewisPublishers.
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 **Duration: 64 Contact hours**
Continuous Assessment: 20 marks **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 appraise 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 Tristhioureacopper(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. ***Tritimetry:***

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

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

i) Silver (Ag^{+}) as AgCl and Nickel (Ni^{2+}) as $[NiEDTA]^{2-}$ complex.

ii) Nickel (Ni^{2+}) as Ni (DMG) complex and Magnesium (Mg^{2+}) as $[Mg\ EDTA]^{2-}$ complex.

iii) Copper (Cu^{2+}) as CuSCN and Magnesium (Mg^{2+}) as $[MgEDTA]^{2-}$ 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 be HCl using polarimeter.

B. Viscometery

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^{th}ed. / 6^{th}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^{th}edn; Jeffery, Bassett; (ELBS, 1989).
4. Quantitative Analysis; 6^{th}edn; Day, Underwood (Printice Hall, 1993).

5. Analytical Chemistry, 6thEd; D. Christian, Wiley.
6. Quantitative Analysis; 6thedn; 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. Comprehensicve 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., Schoemakeret al. , MGH, 1989.

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

Max. Marks: 50 **Duration: 32 Contact hours**
Continuous Assessment: 10 marks **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 OrthoganalityTheorm-elementary idea, consequences of the Great Orthogonolity Theorem. Reducible and Irreducible representations (IRs), Mullikan symbols for IRs, Properties of IRs. Character table-construction of character tables for C2v, C3v and C4v 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 AB2, AB3, AB4, AB5, and AB6 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 **Duration: 32 Contact hours**
Continuous Assessment: 10 marks **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 (N2, O2),

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

Linear harmonic oscillator- classical and quantum treatment of vibrations, vibrational energies ofdiatomic 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; 2nd edn; J L. McHale; CRC Press 2015.
2. Infrared and Raman Spectroscopy; Principles and Spectral Interpretation; 2nd edn.; P. Larkin; Elsevier; 2011.
3. Introduction of Spectroscopy; 4th 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 Spectrsocopy; 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; 1st 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 **Duration: 32 Contact hours**
Continuous Assessment: 10 marks **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 **Duration: 32 Contact hours**
Continuous Assessment: 10 marks **End Term Exam: 40 Marks**

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

- Chemistry involved inWater& 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 Prospective; 2nd edn; Buell and Girad; Jones and Barlett; 2013.
3. www.chemistryincontext; (American Chemical Society)