Course No: CH17304DCE
Title: Laboratory Course in Physical Chemistry (04 Credits)

Max. Marks: *100* — ***Duration:*** *64 Contact hours*
External Exam: *80 Marks.* — ***Internal Assessment****: 20 Marks*

A. Conductometry
1. Determination of the composition of a mixture of HCl and CH_3COOH by titration with standard NaOH.
2. Determination of degree of dissociation of a weak acid.

B. Potentiometry
1. Determination of strength and pKa value of weak acid by titration with an alkali using quinhydrone electrode.
2. Titration of Fe (II) vs. $K_2Cr_2O_7$ and determination of standard redox potential of Fe^{2+}/Fe^{3+}.

C. pH-metry
1. Determination of pKa values of a tribasic acid by titration with an alkali.
2. Determination of degree of hydrolysis of aniline hydrochloride.

D. 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.

E. Spectrophotometry
1. Determination of composition of a binary mixture of $K_2Cr_2O_7$ and $KMnO_4$ or Cobalt (II) and Nickel (II) ions.
2. Spectrophotometric titration of Fe(II) vs. $KMNO_4$.

F. 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.

G. Viscometry
1. Investigation of variation of viscosity with conc. and determination of unknown concentration.
2. Determination of the radius of a molecule by viscosity measurement.

Books Recommended:

1. Practical Physical Chemistry, Findley, Kitchener, Longman, 1977.
2. Advanced Practical Physical Chemistry, Yadav , Goel Pub, 1994.
3. Experiments in Physical Chemistry, 5th ed., Schoemaker et al. , MGH, 1989.

Course No: CH17301CR
Title: Selected Topics in Inorganic Chemistry (04 Credits)

Max. Marks: *100* — ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit Exam:*** *25 marks*
End Term Exam (Units III & IV): *50 Marks*

Unit-I Metal-ions in Biological Systems: (16 Contact hours)

The role of metal-ions in Metal-Protein systems; in trigger and control mechanisms; in structural context; as Lewis acid and as redox catalysts.
Biodistribution and biochemical role of essential trace and ultra-trace elements:- Fe, Zn, Cu, V, Cr, Mn, Ni, P, F and I. Effects of their deficiencies and treatment.
Antagonism and Synergism among essential trace elements.
Alkali and Alkaline earth metal ions (Na^+, K^+, Ca^{2+} & Mg^{2+}): Biological role; ligands and mechanism of ion transport (Facilitated transport, Carriers, Channeling and active transport of Cations).
Role of Lithium in mental health.
Chlorophyll: Structure and role of magnesium in photosynthesis.
Biological Nitrogen Fixation: Dinitrogen Complexes and their reactivity; Nitrogenase enzyme; Fixation via nitride formation.

Unit-II Bonding in Main Group Compounds (16 Contact hours)

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 Compounds (Borazine), Phosphorous–Nitrogen compounds (Cyclophosphazenes, polyphosphazenes and phosphonitrillic halides), Sulphur-Nitrogen compounds (polythiazyls and Sulphur Nitrides)

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 μ_s and μ_{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.
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.

Unit-IV NQR & Mossbauer Spectroscopy. (16 Contact hours)

Basic principles, Spectral parameters such as isomer shift, quadrupole splitting and magnetic splitting, spectrum display.

Application of the technique to the studies of (i) bonding and structure of Fe^{2+} and Fe^{3+} compounds including those of intermediate spin, (ii) Sn^{2+} and Sn^{4+} compounds— nature of M—L bond, coordination number and structure, (iii) detection of oxidation state and inequivalent MB atoms.

NQR isotopes, Nuclear quadruple moment; Electric field gradient; nuclear quadruple coupling constant; Effect of applied magnetic field, Applications.

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; IInd 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. Infrared and Raman Spectra: Inorganic and Coordination compounds ; K. Nakamoto; Wiley.
11. NMR, NQR and Mossbauer Spectrascopy in Inorganic Chemistry ; R.V.Parish; Ellis Horwood.

Course No: CH17302CR
Title: Organic Chemistry (Spectroscopy & Photochemistry) (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (Units III & IV): *50 Marks*

Unit-I Applications of Spectroscopy: (16 Contact hours)

Recapitulation of UV, IR Spectroscopy, Woodward-Fieser rule Characteristic absorptions of various functional groups. Interpretation of IR Spectra.

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. Mass Analyzer Determination of Molecular Formula, Role of Isotopes, Nitrogen Rule, Metastable Peak. Fragmentation pattern like Stevenson rule , initial ionization event, α-cleavage, inductive cleavage, two bond cleavage, Retro-Diels. Alder cleavage, McLaffertey Rearrangements. Fragmentation pattern of alkanes, alkenes, alcohols, phenols, aldehydes, ketones, Carboxylic acids, Amines, Problems based on Mass Spectroscopy. Some specific examples from natural products like flavanoids terpenes, steroids, alkaloids.

Unit-II Nuclear Magnetic Resonance 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 A_2, AB, AX, AB_2, AX_2, A_2B_2. Proton exchange, deuterium exchange, Peak broadening exchange

C-13 NMR : Carbon 13-chemical shifts , proton coupled and decoupled spectra. Nuclear overhouser, Effect, Off-Resonance De-coupling, A quick dip in to DEPT-45 , DEPT-90, DEPT-135.

Introduction to two-dimensional spectroscopy methods, Cosy techniques, HETCOR technique, OESY, combined structure problems.

Unit-III Photochemistry-I. (16 Contact hours)

Photochemical Reactions

Interaction of electromagnetic radiation with matter. Types of excitations. Singlet and triplet states and their lifetimes. Fate of excited molecule: Physical and chemical processes. Transfer of excitation energy: Sensitization and Quenching. Quantum yield. Types of photochemical reactions.

Photochemistry of alkenes

Geometrical isomerisations, cyclisation and dimerisation reactions. Photochemical reactions of 1,3- butadiene (excluding pericyclic reactions). Rearrangements of 1,4 and 1,5- dienes.

Photochemistry of saturated carbonyl compounds

Intramolecular reactions of saturated acyclic and cyclic carbonyl compounds. (Norrish type-I and Norrish type-II processess). Intermolecular cycloaddition reactions (Paterno- Buchi reaction).

Unit-IV Photochemistry –II. (16 Contact hours)

Photochemistry of unsaturated carbonyl compounds

Photochemical reactions of α, β-unsaturated carbonyl compounds. (H-Abstraction and isomerisation to β, γ-unsaturated carbonyl compounds). Photolysis of cyclic α, β-unsaturated ketones (dimerisation and lumiketone rearrangement) and cyclohexadienones.

Photochemistry of Aromatic compounds

Photoinduced isomerisations of benzene and its alkyl derivatives. 1,2 ; 1,3 and 1,4 photoaddition reactions of benzene. Nueleophilic photosubstitution reactions in aromatic compounds. Photo Fries-rearrangement of aryl esters and anilides.

Miscellaneous Photochemical reaction

Photolysis of organic nitrites and their synthetic utility (Barton reaction).

Photochemistry of vision.

Books recommened:

1. Spectrometric identification of Organic Compounds. 5th Ed., R.M.Silverstein, G.C.Bassler and T.C.Morill. (Jhon 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. Intoductory Photochemistry, A.Cox and T.Kemp (McGraw Hall-1971).
6. Organic Photochemistry, 2nd Ed., J.Coxon, and B.Halton (2nd Ed. Cambridge University press-1987).
7. Fundamentals of photochemistry, Rohtagi & Mukherjee (Wiley Eastern-1992).

Course No: CH17303CR
Title: Physical Chemistry (04 Credits)

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

Ist Unit Exam: *25 marks* | ***IInd Unit Exam:*** *25 marks*

End Term Exam (Units III & IV): *50 Marks*

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 pi-bond-order. Alternant hydrocarbons, Naphthalene. 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-Fockself consistent field method. One and two-electron integrals in the light of minimal basis H_2 system

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 Electrochemistry-I (16 Contact hours)

Conductance of electrolyte solutions: Mobility of ions, mobility and conductivity, Einstein relations, dependence of molar conductance on concentration, estimation of K and Λ^0 for weak electrolytes, Theories of Conductance: Debye-Huckel-Onsager conductance equation and brief idea of its extension.

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, recent advances.

Semiconductor electrodes: Structure of seminconductor/electrolyte interface.

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

Theories of Heterogeneous Electron Transfer: Electron transfer at electrified interface at and away from equilibrium. Butller-Volmer equation, low and high field approximations, significance of transfer coefficient.

Electrochemistry in Materials Science: Corrosion, types and mechanism of corrosion, corrosion current, corrosion potential, Electrodics of corrosion in absence of Oxide films; Monitoring and inhibition of corrosion; cathodic and anodic protection, passivation.

Photoelectrochemistry: Band bending across Semiconductor/electrolyte solution interface, photoelectrochemistry across semiconductor/electrolyte interfaces, p-type photocathode, n-type-photoanode, surface effects in photoelectrochemitry, photoelectrochemical splitting of water, photoelectrochemical reduction of CO_2.

Books Recommended:

1. Physical Chemistry –P. W. Atkins, 9th Edition, 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, Tata McGraw 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. M. J. Rosen, J. T. Kunjappu, "Surfactants and Interfacial Phenomena", John Wiley & Sons, New York, 4th Edition, 2012.
7. D. Y. Meyer, "Surfaces, Interfaces and Colloid", VCH Publishers, Inc. 1991.
8. Jonsson, Lindmann, Homberg and Kronberg, "Surfactants and polymers in aqueous solution", John Wiley and sons, 1998.
9. Molecular Thermodynamics of Electrolyte Solutions, Lioyd L Lee, World Scientific, 2008.
10. An Introduction to Aqueous Electrolyte Solutions, Margaret Robson Wright, Wiley, 2007.
11. Modern Electrochemistry 1, 2A,2B 2nd Edition, J. O`M. Bokris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.
12. Electrochemical methods, Fundamentals and Methods, A.J. Bard, L.R. Faulkner, Wiley, 1980.
13. Physical Electrochemistry- Fundamentals, Techniques and Applications, Eliezer Gileadi, Wiley-VCH 2011.
14. Electrochemistry, 2nd Edition, Carl H. Hamann, Andrew Hammett, Wolf Vielstich, Wiley-VCH.

Course No: CH17304DCE
Title: Laboratory Course in Physical Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *80 Marks.* ***Internal Assessment****: 20 Marks*

A. Conductometry
1. Determination of the composition of a mixture of HCl and CH_3COOH by titration with standard NaOH.
2. Determination of degree of dissociation of a weak acid.

B. Potentiometry
1. Determination of strength and pKa value of weak acid by titration with an alkali using quinhydrone electrode.
2. Titration of Fe (II) vs. $K_2Cr_2O_7$ and determination of standard redox potential of Fe^{2+}/Fe^{3+}.

C. pH-metry
1. Determination of pKa values of a tribasic acid by titration with an alkali.
2. Determination of degree of hydrolysis of aniline hydrochloride.

D. 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.

E. Spectrophotometry
1. Determination of composition of a binary mixture of $K_2Cr_2O_7$ and $KMnO_4$ or Cobalt (II) and Nickel (II) ions.
2. Spectrophotometric titration of Fe(II) vs. $KMNO_4$.

F. 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.

G. Viscometry
1. Investigation of variation of viscosity with conc. and determination of unknown concentration.
2. Determination of the radius of a molecule by viscosity measurement.

Books Recommended:

1. Practical Physical Chemistry, Findley, Kitchener, Longman, 1977.
2. Advanced Practical Physical Chemistry, Yadav , Goel Pub, 1994.
3. Experiments in Physical Chemistry, 5th ed., Schoemaker et al. , MGH, 1989.

Course No: CH17305DCE
Title: Chromatographic Techniques (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*

Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

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; 5th Edition; F. W. Fifield, D. Kealey; Blackwell Sciences Ltd.; 2000.
2. Modern Analytical Chemistry; David Harvey; McGraw-Hill; 2000.
3. Chromatographic Methods; 5th edn. ; A. Braithwaite and F. J. Smith; Kluwer Academic Publishers.
4. Fundamentals of Analytical Chemistry; 6th 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: CH17306DCE
Title: Non-Equilibrium Thermodynamics (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

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 stationery 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 IrreversibleProcesses;DeGroot,Mazur;Dover;1986.
2. Introduction to Thermodynamics of Irreversible Processes; I.Prigogine; Wiley Interscience; 1967.
3. Thermodynamics for students of Chemsitry, Kuriacose, Rajaram, (S. ChandandCo., 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-equlibrium thermodynamics, 2^{nd} ed. Yasar Demirel. Elsevier, 2007.

Course No: CH17307GE
Title: Industrial Pollution and Green Chemistry (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Industrial Pollution and Environmental Toxicology (16 Contact hours)

Industrial Pollution: Cement, Sugar, Drug, Paper and pulp. Thermal power plants, Nuclear power plants and Polymers.

Radio nuclide analysis: Disposal of wastes and their management.

Principles of Toxicology, Dose Response Relationship, risk assessment and management.

Organochlorine Compounds: Accumulation and fate in biological systems. Toxicology of PCBs. Dioxins and Furans, Health effects in humans.

Environmental Estrogens.

Unit-II Green Chemistry (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 and Sonication.

Green Solvents and Reaction conditions: Supracritical fluids, aqueous reaction conditions, immobilized Solvents and irradiative reaction conditions.

Examples of Green materials, reagents and some specific reactions.

Books Recommended

1. Environmental Chemistry; 8^{th} edn.; S. E. Manahan; CRC Press; 2005.
2. Chemistry of the Environment; IInd edn.; T. G. Spiro and W. M. Stigliani; Prentice Hall; 2002.
3. Environmental Chemistry; IInd edn.; Colin Baird; Freeman & Co.; 1991.
4. Chemistry of the Environment; IInd Edn. R. A. Bailey; H. M. Clark; J. P. Ferris; S. Krause & R. L. Strong; Elsevier; 2005.
5. Environmental Chemistry; IInd edn.; Samir K. Banergi; Prentice- Hall; 2001.
6. Green Chemistry- Environment Friendly Alternatives; Rashmi Sangh & M. M Srivastava; Narosa; 2007.
7. Green Chemistry- An Introductory Text; IInd Edn.; Mike Lancaster; RSC; 2010.
8. Green Chemistry- Theory and Practice; P. T. Anastas and J. C. Warner; oxford; 2000.
9. Green Chemistry; Ist Edn.; Samuel Delvin; IVY Publishing House; 2008.
10. Green Chemistry- Environmentally Benign Reactions; V. K. Ahluwalia; Ane Books; 2006.

Course No: CH17308GE
Title: Bio-Organic Chemistry (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I (16 Contact hours)

(a) Chemical Origins of Biology

Bio organic chemistry: Introduction ,Basic consideration , Proximity effects in Organic Chemistry , Molecular rearrangments.

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 Nomeclature 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+ and NADP+), Flavin Nucleotides (FMN and FAD), Adenosine phosphate (ATP, ADP, AMP) .

Coenzyme A (CoA -SH) ,Thiamine Phosphate, Biotin, Tetrahydrofolate, Coenzyme B_{12} .

(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 Gregary Weiss; Taylor and francis. 2013.
2. Bio-organicchemistry : Harman Dugas 3rd ed.Springer (2010) .
3. Bio-organic chemistry J.Rohr ,Springer (2000).
4. Enzymes 2nd ed. T. Palmer and P. Bonner (2008).
5. Biochemistry :Donald Voet, Judith.G. Voet 2nd ed.Willey (1995)

Course No: CH17309OE
Title: Philosophy of Science (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*

Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Representation (08 contact hours)

Laws of nature**:** Knowledge**, S**ources of knowledge, The rationalists, The empiricists, The Mathematical knowledge, Synthetic Knowledge, Science as knowledge source, Religion and science The Method of science, Induction versus deduction, Representation and reason, Probabilistic laws, Basic and derived laws,

Realism: Realism and its critics, Instrumentalism, Constructive empiricism, Laws and antirealism, Anti-realism and structure of science.

Unit-II Reason (08 contact hours)

Inductive Scepticism: Theory and observation, Dissolving the problem of Induction, Probability
and scientific inference, Kinds of Probability,

Inductive Knowledge: Reliabilist epistemology, reasoning with induction, Innate epistemic capacities and reasoning about induction, Internalism and justification.

Method and Progress: Methodology of scientific research programmes, Clinical trials and the scientific method, The content of discovery and the context of justification, Science without the scientific method, Method and the development of sciences, Paradigms and Progress.

Unit-III Classical Determinism and Probabilistic world (08 contact hours)

The Classical Mechanics: Mechanistic determinism, General principles; Action at a distance, Electric and magnetic forces, Failures of the classical mechanics;
Atomic structure, problem of radiation.

The birth of modern science**:** The photo-electric effect**,** The atomicity of radiation, Particle wave duality, waves of probability, Uncertainty principle, subject versus object, the fundamental laws of radioactivity, The new Quantum theory, wave mechanics, Diracs Quantum mechanics, The new philosophical principles, the probabilistic reasoning.

Unit-IV The Dawn of Modern Thinking (08 contact hours)

The arrow of Time: From Descarts to quantum theory, the relation of quantum theory to other natural sciences. Language and reality in modern science. The role of modern science in the present development of human thinking.

Books Recommended:

1. Philosophy of science; Alexander Bird; McGill-Queen's University Press.
2. Physics and Philosophy; W. Heisenberg; Harper Perennial Modern Classics.
3. Physics and Philosophy; Sir James Jeans; Cambridge University Press.
4. Reconstruction of religious thought in Islam; Muhammad Iqbal; Adam Publishers & Dodo Press.
5. Philosophy of natural science; Carl G. Hempel**;** Pearson.
6. The philosophy of science; David Papineaus; Oxford University Press.
7. Reality and Representation; David Papineaus; Blackwell Publication.
8. Belief, truth and knowledge; D.M. Armstrong; Cambridge University Press.
9. Modern epistemology; Nicholas Everitt and Alec Fisher; McGraw-Hill Higher Education.
10. The structure of scientific revolution; Thomas S. Kuhn; The University of Chicago Press

Course No: CH17401CR
Title: Organo-Transition Metal Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Sigma Bonded Organometallic Compounds: (16 Contact hours)

Classification, Stability, Comparison to main Organometallic Compounds, Routes of synthesis, Reactions. Decomposition Pathways: Choice, α and β hydrogen transfer. Intramolecular elimination of alkane, Cyclometallation, Stability from bulky substituents, Agostic alkyls, Umpolung.Metal Hydride Complexes: Synthesis, Characterization and Chemical reactions, Non-classical Hydrides (Kubas complexes).

Unit-II Pi-bonded Organometallic Compounds: (16 Contact hours)

Classification, Structure and bonding in Metal- alkene, alkyne, allyl, 1,3-butadiene and Cyclobutadiene Complexes.

Sandwich Compounds: Characteristics; Classification, Synthesis, Reactions, 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.

Unit-III Catalytic Processes involving Transition Metal Organometallic Compounds: (16 Contact hours)

Mechanistic aspects: Oxidative addition, Insertion reactions Reductive elimination and water gas shift reaction (WGSR).

Catalytic mechanism of Hydrogenation, Hydroformylation, Oxidation and Isomerization of alkenes; Olefin metathesis.

Fischer-Tropsch Synthesis and Ziegler Natta polymerization of alkenes.

Asymmeteric and supported Organometallic Catalysis (brief idea)

Unit-IV Fluxional Organometallic Compounds and Synthetic Reactions involving Organo- metallics (16 Contact hours)

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 η^1 Cyclopentadienyls and η^3–allyls.

Stereochemical non rigidity in case of coordination numbers- 4 & 5 (cis-trans, atomic inversion, Berry Pseudorotation).

Synthetic Reactions involving Organo- metallics:

Reactions of coordinated ligands, carbon monoxide, alkyls, alkenes (Green, Mingo’s rules).

Activation of small molecules: Carbon monoxide, Carbon dioxide and Alkanes.

Role of organo-iron as synthons, Carbon-Carbon coupling and its reactions (Suzuki and Heck).

Books Recommended:

1. The Organometallic Chemistry of Transition Metals; 2nd edn; Robert. H . Crabtree; Wiley; 1994.
2. Fundamental Transition Metal Organometallic Chemistry; Luke hart; Brooks / Cole; 1985.
3. Organometallic Chemistry; 2nd edn ; Mehrotra & Singh ; New age international 2000
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 press 1983.
9. Reaction Mechanism of Inorganic and Organometallic systems; 2nd edn.; Robert .b. Jordan 1998.
10. Inorganic Chemistry ; 4th edn.; Huheey ; E. Keiter & R. Keiter; Addison-Wesley ;1983
11. Modern Inorganic Chemistry; William. A. Jolly; McGraw Hill; 1985.

Course No: CH17402CR
Title: Photo-Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Basics of Photo-Chemistry (16 Contact hours)

Absorption; mechanism of absorption of light

Transition moment integral, Einstein's treatment, molar integrated absorption intensity, natural radiative lifetime & the calculation of life times.

Excitation; d-d transition, charge transfer & intraligand 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 diagramsdepicting excited states.

Frank Condon principle, shapes of absorption & emission bands.

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

Tools and Technique: Light source, measurement of light intensity, chemical actinometry. Flash photolysis.

Unit-II The Chemistry of Excited State Molecules (16 Contact hours)

Photochemical laws & quantum yield. Kinetics & quantum yield of photo-physical (radiative) and photo-chemical processes. Photochemical processes: primary, secondary, adiabatic & non- adiabatic. Properties of thexi states; Determination of dipole moments & acidity constants of excited state molecules.

Photosubstitution and photo reduction of Co (III) complexes.Photosubstitution reaction of Cr (III) and Rh (III) complexes.

Organometallic-Photochemistry: Reactions of metal carbonyls, cleavage of metal-metal bond.

Unit-III Redox Reactions by Excited Metal Complexes (16 Contact hours)

Energy transfer under conditions of weak and strong interaction. Excited state electron transfer. Marcus-Hush model.Conditions of the excited states to be useful as redox reactants. Photochemical electron transfer, [Ru (bipy)3]2+ and [Os (bipy)3]2+.

Photochemical supramolecular devices: devices for photo-induced energy or electron transfer, Devices for information processing, photo-chemically driven molecular machines.

Unit-IV Solar Energy-Prospects and Challenges (16 Contact hours)

Solar energy storage, solar energy conversion, Metal complex sensitizers and electron relays in photochemical splitting of water, Nitrogen fixation and CO_2 reduction. Inorganic photolithography.

Supramolecular photochemistry in natural systems: photosynthesis, bacterial photosynthesis and artificial photosynthesis.

Books Recommended:

1. Reaction Mechanisms of Inorganic and Organometallic Systems; 2nd edn.; Jordon; Oxford; 1998.
2. Mechanism of Inorganic Reactions; Katakis, Gordon; Wiley; 1987.
3. Inorganic Chemistry; 4* edn; Huheey; Harper & Row; 1990.
4. Mechanism of Inorganic Reactions, 2nd edn, Basalo, Pearson; Wiley Eastern, 1997.
5. Chemistry of Light; Suppan, Royal Society; 1994.
6. Photochemistry, Carol J. Wayne and Richard P. Wayne; Oxford University Press; 1996.
7. Fundamentals of Photochemistry; C Rohatgi, Mukhergi; Wiley Eastern.; 1992
8. Inorganic Photochemistry; J.Chem Edu.;Vol .60, No.10,1983.
9. Applications of Inorganic Photochemistry; J. Chem. Edu.; Vol.74, No 69. 1997.

Course No: CH17403CR
Title: Bio-Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Iron Storage, Transport and Oxygen carriers: (16 Contact hours)

Structure and Coordinating sites in biologically important ligands: Proteins, Nucleotides and Lipids.

The transport mechanism: uniport, symport and antiport.

Ferritin and Transferrin: Structure, Metal binding sites; incorporation and release of iron.

Porphyrins: Introduction, characteristic absorption spectrum and salient characteristics.

Haemoglobin and Myoglobin: Structure, oxygen saturation curves; Mechanism of oxygen transport and storage.Bohr effect and cooperativity in haemoglobin.

Hemerythrin and Hemocyanin: Structure, Metal binding groups and Dioxygen binding. Synthetic oxygen carrier model compounds: Vaska's iridium complex: Cobalt complexes with micro and macrocyclic ligands and Schiff base ligands.

Unit-II Metallo-enzymes and Electron Carriers (16 Contact hours)

Enzyme, Apoenzyme, Coenzyme, Prosthetic group and Metalloenzymes, Mechanism of enzyme action.

Zinc enzymes:- Carboxypeptadiase and Carbonic Anhydrase : Introduction, Structure, Mechanism of action and their model compounds.

Biological chemistry of Molybednum: uptake of Molybednum; oxidation states and redox potentials in enzymes and oxygen atom transfer reactions.

Xanthine oxidase and Aldehyde oxidase: Structure and biological role.

Cobalt in Vitamin B_{12}: Introduction, Structure and Derivatives of B_{12} and mechanism of alkylation reaction. Role of vitamin B_{12}.

Electron Carriers: Rubredoxin & Ferridoxin (Structure and biological role).

Blue Copper proteins: Oxidases and Plastocyanin (Structure and biological role).

Unit-III Metal-ion Induced Toxicity and Chelation Therapy (16 Contact hours)

Toxic levels of different metals. Sources of metal ion poisoning (external sources and internal disorders).

Mechanism of metal ion induced toxicity:- Toxicity of Pb, Cd, Hg, As, and CN- Metal ion promoted Carcinogenesis and probable mechanism of action.

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 Metal Salts and Metal Complexes in Therapeutics (16 Contact hours)

Treatment of essential metal deficiencies: Iron, Copper and Cobalt.Metal salts as anti-acids, antiseptic and diuretics.

Gold compounds and Rhematoid arthiritis.

Anti-Cancer Drugs: cis-Platin and its derivatives. Structure-function relationship.

Complexes of Rhodium, Gold and Cobalt.

Anti-bacterial, Anti-viral and Anti-fungal activities of Metal Complexes: Labile and Robust metal complexes; Probable mechanism of action.

Books Recommended:

1. As listed for Course No. CHM—101 (Inorganic chemistry-M.Sc. 1st Semester! From serial No. 1 to 5.
2. Bio inorganic Chemistry -An introduction; Ochai, Allyn and Bacon; 1977.
3. Inorganic Bio-chemistry—Vol. 1&2; Eichhorn; Elsevier, 1973.
4. Inorganic Aspects of Biological and Organic Chemistry; Hanzilik; Academic; 1976.
5. The Inorganic Chemistry of Biological processes; 2nd edn.; Hughes ; Wiley; 1973.
6. A Text book of Medicinal aspects of Bio inorganic Chemistry; Das; CBS; 1990.
7. The Biological Chemistry of Elements; Frausto de Silva; Williams; Clarenden; 1991.
8. Principles of Bio inorganic Chemistry; Lippard, Berg; Univ. Science Books; 1994.
9. Inorganic Chemistry in Biology; Wilkins C & Wilkins G; Oxford; 1997.
10. Bio inorganic Chemistry ; K. Hussain Reddy; New Age International (P) Ltd; 2005.
11. Metal -Ions in Biochemistry; P. K. Bhattacharya; Narosa Publishing House; 2005.

Course No: CH17404CR
Title: Heterocyclic Chemistry (04 Credits)

Max. Marks: *100* | ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Structure and Nomenclature of Heterocyclic compounds (16 Contact hours)

Introduction and significance of heterocycles in day to day life.

Nomenclature of Heterocycles: Monocyclic, bicyclic and polycyclic heterocycles, Hantzsch-Widman and replacement methods of nomenclature.

Structural features: Non-aromatic, aromatic and heteroaeromatic heterocycles.

Tautomerism in heterocycles, Meso-ionic systems.

Spectroscopic properties of heterocycles (UV,Visible and ^{1}HNMR).

Unit-II General Approach to Synthesis of Heterocyclic compounds (16 Contact hours)

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 quinoline, Bischler-Napieralki Isoquinoline,Knorr Pyrrole,Paal-Knorr , Fischer – Indole synthesis.

Unit-III Monocyclic Heterocycles (16 Contact hours)

Structure, Synthesis and Reactions of Oxirane, Thirane, Azetidine, Pyrrole, Furan, Thiophene, Diazenes, Pyrimidines,Pyridine.Chemistry of five membered heterocycles with two heteroatoms like 1,3-Azoles, 1,2- Azoles. Chemistry of Six membered rings like Azines and seven membered heterocycles like Azepine,Oxipene,Thiepins.

Unit-IV Bicyclic Heterocycles (16 Contact hours)

Structure, Synthesis and reactions of Benzo- fused heterocycles like Benzo-pyrrole, Benzo-furan,Benzo-thiophene, Quinoline, Isoquinoline, Chromones, Coumarins, Iso-Coumarins, 2 and 4-benzopyrones, Benzopyryllium salts and purines.

Books Recommended:

1. Heterocyclic Chemistry, 5th Ed. J.A.Joule and K.Mills, (Wiley-2010).
2. Essentials of Organic Chemistry, Paul M Dewick , (Wiley-2006).
3. Heterocyclic Chemistry, J.A. Joule and G.F.Smith , (Chapman and Hall-1996).
4. The Chemistry of Heterocycles Theophil Eicher and Siegfried Hauptmann , (George Thieme Verlag Stutt gart,New York -1995).
5. Heterocyclic Chemistry, Raj K. Bansal, (New Age International Publisher-2006).
6. Heterocyclic Chemistry, R.R.Gupta,M.Kumar,V.Gupta,(Springer-2006).

Course No: CH17405CR
Title: Chemistry of Natural Products (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Terpenoids and Carotenoids (16 Contact hours)

Introduction, classification, general methods of isolation, separation.

Essential oils: Separation using Gas Liquid Chromatography and High Performance Liquid Chromatography. Physical, chemical and spectral methods of structure elucidation.

Structure determination, stereochemistry and synthesis of α-terpineol, abietic acid and β-carotene.

Unit-II Alkaloids (16 Contact hours)

Introduction, classification, nomenclature, qualitative tests, pharmaceutical applications and general methods of isolation. Physical, Chemical & Spectral methods of structure elucidation.

Stereochemistry, synthesis and biosynthesis of Quinine, Morphine and Reserpine.

Unit-III Steroids (16 Contact hours)

Introduction, nomenclature, classification & stereochemistry. Physical, Chemical & Spectral methods of characterization. Qualitative tests.

Cholesterol: Isolation, clinical significance, chemical properties, structure elucidation, total synthesis & relationship with bile acids.

Sex hormones: Introduction, isolation, clinical & commercial significance, color reactions, structure determination and partial synthesis of Oesterone, Androsterone, Testosterone and Progesterone.

Glucocorticoids & Mineral Corticoids: Introduction and partial synthesis of Cortisone, aldosterone and synthesis of cholecalciferol.

Unit-IV Natural Plant Pigments and Porphyrins (16 Contact hours)

Introduction, classification, physical, chemical, degradative and spectral methods of structure determination and biosynthesis (Acetate and Shikimic acid pathway)

Flavonoids: Isolation, separation and quantification. Antioxidant activity of flavonoids. Robinson's synthesis, Baker Venketraman synthesis, Kostanecki synthesis of flavanone and Flavanol.

Isolation, structure determination and synthesis of Cyanidin, Chrysin, Quercitin & Genestein.

Porphyrins: Structure determination and total synthesis of haemoglobin. Structural comparison with chlorophyll.

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. New Trends in Natural Product Chemistry, Atta-ur-Rahman (Harward Academic Press).
4. Chemistry of Natural Products, N.R. Krishnaswamy (University Press-1999).
5. Flavanoids; Oyvind M. Andersen and Kenneth R. Markhan. (Taylor & Francis -2006)

Course No: CH17406CR
Title: Bio-Organic and Medicinal Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

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

Vitamins:_ Source, structure and synthesis of vitamins – Vitamin A, Vitamin B-Complex (Thiamine riboflavin, folic acid); Vitamin B-12 (Structure only) Vitamin C, E, K, H and D.

Prostaglandins : Introduction and nomenclature, approaches to prostaglandin synthesis, cyclo-hexane, precursors-Woodward synthesis of PGF2a. Cyclo-heptane precursors - Corey's synthesis of prostoglandin's E & F.Their relationship with oxygenase I and II.

Nucleic Acids: Structure of nucleotide, nucleosides, RNA and DNA, role of nucleic acids in protein synthesis, genetic code and heredity. DNA finger printing

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

Enzymes : Introduction, nomenclature & classification.. Activation & inhibhion of enzymes. Mechanism of enzyme action- Fischer lock and key, koshlands induced fit hypothesis, displacement reactions & coupling of ATP. Enzyme mechanism of chymotrypsin lysozyme & carboxypeptidase.

Co-Enzymes: Cofactors derived from vitamins, coenzymes, prosthetic groups. Apoenzyme. Structure , biological function and mechanism of reactions catalsed by co-enzymes: coenzyme A, thiamine pyrophosphate. pyridoxal phosphate, NAD+, NADP+, FMN, FAD and Lipoic acid.

Unit-III **(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, carbonylic, thiols sulphides groups and introdction/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. Lipophillic constant, Hamett constant, steric parameters and Hansch analysis.

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

Antibiotics: Classifications-structural and mechanistic, cell wall biosynthesis inhibitors, protein synthesis inhibitors. Pencillins-classification and structures. Synthesis of Pencillins, V, G, chloroamphenicol.and ciprofloxacin. Tetracyclins.

Psychoactive Drugs: Introduction, CNS depressants, CNS stimulants, sedatives and hypnotics, barbutirates. Synthesis of diazepam, phenytoins and glutethisimide.

Anti-neoplastic drug: Introduction; cancer chemotherapy, carcenoolytic antibiotic, plant derived anti-cancer agents (Taxol)role of alkylative agents and antimetabolites in treatment of cancer, mitotic inhibitors (elementary idea).

Cardiovascular Drugs: Introduction, cardiovascular diseases, synthesis of Amylnitrate. sorbitrate, quinidine, verapanil, methyl dopa and atenolol

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, Biotechonolgy and Clinical Chemistry of Enzmyes. Trevor Palmer (EWP)
5. Organic Chemistry by I.L.Finar Vol. II (ELBS Longamnn)
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. Chemsitry of Natural Products. S.V. Bhat, B.A. Nagasampagi, M. Siva Kumar. Naroosa Publishing House, New Delhi.

Course No: CH17407CR
Title: Advanced Quantum Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Electronic Structure Theory, Hartree-Fock Method (16 Contact hours)

Review: Electronic Hamiltonian, antisymmetrized wave function, Slater determinant. Hartree-Fock self-consistent field method. One and two-electron integrals in the light of minimal basis H_2 system.

Hartree-Fock Equation, Fock, Coulomb and exchange operators and integrals, restricted Hartree-Fock formalism, Roothaan equation. The Fock matrix elements, Koopman's theorem, Slater-Condon rules. Matrix form of Roothaan equation, the SCF procedure.

Basis Sets: Slatter-type orbitals, Gaussian basis sets. Model SCF calculations on H_2 /HeH^{+}.

Unit-II Configuration Interaction and Semiempirical methods (16 Contact hours)

Configuration Interaction: Electron correlation, configuration state functions, configuration interaction (CI), Brillouin theorem, full and truncated CI theories- CID, CISD, CISDTQ methods; Size consistency problem. Moller-Plesset and Coupled Cluster methods.

Semiempirical methods: The ZDO approximation; the PPP method, brief idea of CNDO, INDO and NDDO methods. The MINDO, MNDO, AM1 and PM3 methods.

Unit-III Density Functional Methods and Molecular Properties (16 Contact hours)

Density Functional Theory:Electron probability density. Hohenberg-Kohn theorems, Kohn-Sham formulation of DFT, n- and v- representabilities, E_x&$E_c$functionals; the local density and local spin density approximations, gradient corrected and hybridfunctionals.

Brief idea of Molecular mechanics methods, force fields.

Molecular Properties*:* Potential energy surfaces; molecular geometry and its optimization, Hessian Matrix and normal modes, vibrational frequencies, thermodynamic properties. Dipole moments, atomic Charges.

Unit-IV Use of Quantum Chemistry Software: Gaussian (16 Contact hours)

A quick tour of GAUSSIAN Interface. Input to Gaussian. Model calculations illustrating various features of the package**..**

1. A single point energy calculation: HCHO /CH3.CHO,HCHOMOs.
2. Geometry Optimization: Input and Output for ethene, fluoroethene, propene conformers
3. Transition state optimization $CH_2O \rightarrow HCOH$
4. NMR properties of ethane, ethene and ethyne.
5. Frequency Calculations: Input, Formaldehyde frequencies, Normal modes, zero point energy, thermodynamic properties, polarizability, hyperpolarazability.
6. Stationary points characterization –C3H5F
7. Model Chemistries: Basis set effect on HF bond length

8. Selecting an appropriate theoretical method:
   a) Electron correlation and post SCF methods, limitations of Hartree-Fock theory: HF bond energy, Optimization of O_3.
   b) Density Functional Theory: CO_2 structure and atomization energy.
   c) Butane / Isobutane isomerization energy, rotational barrier in n-butane.

9. Chemical reactions and reactivity:
   a) Hydration enthalpy of the reaction $H^+ + H_2O \rightarrow H_3O^+$
   b) Potential energy surfaces. Reaction path following (IRC calculation)
   $CH_2O \rightarrow HCOH$
   c) Heat of formation of CO_2 via an isodesmic reaction
10. Solvation models: Formaldehyde Frequencies in Acetonitrile

Books Recommended

1. Quantum Chemistry, Ira. N. Levine, (Prentice Hall, 2009).
2. Quantum Chemistry, 2nd Edn , D. A. McQuarrie, (University Science Books, 2007).
3. Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedmann, (Oxford, 2008).
4. Quantum Chemistry and spectroscopy, Engel & Reid, Pearson (2007)
5. Modern Quantum Chemistry - Introduction to Advanced electronic structure theory - A. Szabo & N. S. Ostlund, (Macmillan, 1982, Dover 1996).
6. Molecular Modeling, Principles and Applications, A. R. Leach, Prentice-Hall, 2001
7. Modern Electronic Structure Theory, D. R. Yarkouy (ed). (World Scientific, 1995)
8. Ab Initio Molecular Orbital Theory, by Hehre, Radom, Schleyer and Pople, (Wiley)
9. Density Functional Theory of Atoms and Molecules, R.G. Parr and W. Yang, Oxford(1989).
10. GAUSSIAN Manual, Gaussian Inc
11. Exploring chemistry with electronic structure methods, Foresman J.B., Frisch A., Gaussian Inc

Course No: CH17408CR
Title: Advanced Electrochemistry and Statistical Mechanics (04 Credits)

Max. Marks: *100* | ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Instrumental Methods in Electrochemistry (16 Contact hours)

Fundamentals: Electrode potential and its measurement, standard and formal electrode potentials, three electrode measurements, uncompensated resistance.

Overview of electrode Processes: Faradaic and Non-Faradaic processes, factors affecting electrode reaction rate. Mass transfer: Convection, migration, diffusion, Fick's 1st and 2^{nd} law of diffusion,

Electrochemical Techniques:

Electrophoresis: Factors affecting ion migration, electro-osmosis, theory and applications of capillary electrophoresis.

Potential Step Methods: Chronoamperometry, Chronocoulometry at macro electrodes; theory and applications. Cottrell equation. Controlled-Potential coulometry, Constant-Current coulometric titrations.

Potential Sweep Methods: Linear sweep Voltammetry and Cyclic Voltammetry at macro electrodes theory and applications, Diagnostic criteria of Cyclic Voltammetry.

Unit-II Applied Electrochemistry (16Contacthours)

Electrochemistry of redox enzymes: Direct and mediated electron transfer, Enzyme modified electrodes-challenges and applications. Mechanism and approach to bioelectrosynthesis, examples of bioelectro synthesis-oxidation of alcohols, synthesis of dihydroxy acetone phosphate, site specific oxidation of sugars, reduction of carbonyl compounds, hydrogenation.

Energy storage devices: Desirable characteristics of energy storage devices, Discharge plot, Ragone plot. Batteries: Measures of battery performance. Classical batteries (Lead Acid, Nickel-Cadmium, Zinc-Mangenese dioxide). Modern batteries (Zinc-Air, Nickel-Metal Hydride, Lithium Ion Batteries), Supercapacitors.

Fuel cells, types of fuel Cells, basic fuel cell operation, kinetics of fuel cell reactions. Alkaline, Phosphoric acid, Polymer Electrolyte membrane and direct MeOH fuel cell, biofuel cells.

Unit-III Classical Statistical Mechanics and Ensemble concept (16 Contact hours)

Equations of Motion; Newton, Lagrange and Hamiltonian. Classical partition function, phase space and the Liouville equation, Kinetic theory of gases, equi-partition of energy, Maxwell's velocity distribution.

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. Statistical Mechanical treatment of imperfect gases. Virial equation of state from grand

partition function, virial coefficients in the classical limit, second and third virial coefficients.

Unit-IV Applied Statistical Mechanics (16 Contact hours)

Quantum Statistics: Fermi-Dirac and Boson-Einstein statistics, Nuclear spin statistics, symmetry and nuclear spin, Ortho and Para nuclear spin states, Ortho and Para Hydrogen and Deuterium, CO.

Application of grand partition function to Boson-Einstein and Fermi-Dirac statistics. Ideal Fermi-Dirac gas: Electrons in metals, Ideal Photon gas: Black body radiation, influence of wavelength for the Planck distribution, Bose-Einstein condensation.

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. Electrochemical Methods Fundamentals and Applications, 2ndEdition, Allen J.Bard, Larry R. Faulkner, John Wiley and Sons, INC.
2. Physical Electrochemistry-Principles, Methods and Applications, Israel Rubinstein (Ed.) Marcel Dekker, Inc. New York.
3. Understanding Voltammetry, 2nd Edition, Imperial College Press.
4. Elements of Molecular and Biomolecular Electrochemistry, Jean-Michel Saveant, Wiley-Interscience.
5. Electrochemistry, 2nd Edition, Carl H. Hamann, Andrew Hammett, Wolf Vielstich,Wiley-VCH.
6. Modern Electrochemistry 2B, 2nd Edition, J. O`M. Bockris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.
7. Statistical Thermodynamics, M. C.Gupta ,(NewAgeInternational,1993).
8. Statistical Thermodynamics-Fundamentals and Applications, N.M. Laurendeau, Cambridge University Press, 2005.
9. Statistical Mechanics, D.A. McQuarrie, (Viva,2003).
10. Introduction to Statistical Thermodynamics, Chandler, (OUP, 1987).
11. Statistical Thermodynamics and Kinetic Theory, C. E. Hecht, (Dover,1990).
12. Statistical Mechanics –Principles and Applications, Hill, Dover, 1987.
13. Statistical Thermodynamics for Chemists, A. Ben-Naim, (Plenum, 1992).
14. An introduction to Statistical Thermodynamics, Hill, (Addison-wesley,1987).

Course No: CH17409CR
Title: Chemistry of Materials (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Surfactant mixtures, Stimuli responsive surfactants and block copolymers (16 Contact hours)

Surfactant-Surfactant Interactions: Mixed micelle formation, mixed monolayer formation, synergism, Clint and Rubingh's models of mixed micelle formation**.** Importance and practical applications of mixed surfactant systems.

Stimuli-Responsive Surfactants: Introduction and applications: Biosurfactants, redox, photochromic, thermoreversible, pH-sensitive, cleavable and magnetic surfactants.

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

Unit-II Hydrogels and microemulsions (16 Contact hours)

Hydrogels: Introduction, Types of Hydrogels, Preparation, Properties and characterization of Hydrogels, Biomedical applications of Hydrogels.

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

Unit-III Langmuir Blodgett Films, Liquid crystals and Fullerenes (16 Contact hours)

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.

Fullerenes: Fullerenes- History, bonding, properties, doped fullerenes, fullerenes as superconductors and fullerene related compounds (carbon nanotubes).

Unit-IV Optical materials and Ionic conductors (16 Contact hours)

Optical materials: Luminesence and phosphors. Lasers – general principle of lasing action, Ruby laser, Neodymium-YAG lasers, semiconducing lasers and quantum dot lasers. Nonlinear optical effects, second and third order harmonic generation, nonlinear optical materials.

Ionic Conductors: Introduction to ionic conduction and mechanism. Types of ionic conductors, mechanism of ionic conduction, interstitial jumps (Frenkel); vacancy

mechanism. Super-ionic conductors: Diffusion and transition superionic conductors and mechanism of conduction in superionic conductors; examples and applications of ionic conductors.

Books Recommended:

1. M. J. Rosen, J. T. Kunjappu, “Surfactants and Interfacial Phenomena”, John Wiley & Sons, New York, 4^{th} Edition, 2012.
2. R. D. Vold and M. J. Vold, “Colloid and Interface Chemistry”, Addison-wesley, 1982.
3. .D. Y. Meyer, “Surfaces, Interfaces and Colloid”, VCH Publishers, Inc. 1991.
4. Jonsson, Lindmann, Homberg and Kronberg, “Surfactants and polymers in aqueous solution”, John Wiley and sons, 1998.
5. D. Fennell Evans, H. Wennerstrom, “The Colloidal Domain where physics, chemistry, biology and technology meet” VCH, New York, 1994.
6. Robert J. Hunter, “Foundations of Colloid Science”, Oxford University Press, New York, 2007.
7. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
8. I. W. Hamley, The Physics of Block Copolymers (Oxford University Press, Oxford, 1998.
9. N. Hadijichristidis, S. Pispas and G. A. Floudas Block Copolymers (Wiley, New York, 2003).
10. Introduction to Solids, Azaroff, Tata McGraw,1993.
11. SolidState Chemistry and its Applications, West, Wiley,1989.
12. The Physical Chemistry of Solids, Borg, Biens, Academic press, 1992.
13. Solid State Physics, N. W. Ashcroft and N. D. Mermin, Saunders college, 2001
14. Principles of Solid State, H. V. Keer, Wiley Eastern.
15. The Physics and Chemistry of materials, J.I. Gersten, F.W. Smith, John Wiley and sons, Inc. 2001.
16. Microemulsions: Background, New Concepts, Applications, Perspectives, C. Stubenrauch, Blackwell Publishing Ltd, 2009.
17. M. Sirousazar, M. Foroug, K. Farhad, Y. Shaabani and R. Molaei, Hydrogels: Properties, Preparation, Characterization and Biomedical, Applications in Tissue Engineering, Drug, Delivery and Wound Care, IN Advanced Healthcare Materials, Wiley online Library, 2014.

Course No: CH17410DCE

Title: Advanced Laboratory Course in Inorganic Chemistry (04 Credits)

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

External Exam: *75 Marks.* ***Internal Assessment****: 25 Marks*

A: - Inorganic Preparations: (5 Experiments)

- Preparation of tetraamminecarbonatocobalt (III) nitrate and its conversion to pentaamminecholorocobalt (III) chloride.
- Preparation of trans dicholoro bis (ethylenediamine) cobalt (III) chloride and its conversion to cis-isomer.
- Preparation of tris (ethylenediamine) nickel (II) chloride dihydrate and its conversion to bis (ethylenediamine) nickel (II) chloride.
- Preparation of bis (acetylacetonato) copper (II) dihydrate.
- Preparation of pentaamminecholorocobalt (III) chloride and study of Linkage isomers by its conversion to pentaamminenitritocobalt (III) chloride and to nitro isomer followed by IR Characterization.

B:- Total analysis of a Coordination compound for determination of various components present.

(1- Experiment)

C: - Separation by Column Chromatography and Estimations: (5 Experiments)

- Separation of Permanganate and Bichromate ions on Alumina column and their Estimation from Beer Law plots.
- Determination of lonisable chloride in a Complex by cation exchange column (separation followed by Mohr's titration of elute for estimation).
- Separation of Cobalt (II) and Nickel (II) on anion exchange column followed by estimation through EDTA titrations.
- Separation of two Cobalt (III) complexes viz $[Co(NH_3)_6] Cl_3$ and $[Co (NH_3)_5 Cl] Cl_2$ on Silica column.
- Ion exchange separation of Hydration / ionization isomers of Chromium (III) Chloride ($CrCl_3$).

D: - Potentiometric Titrations: (6 Experiments)

- Standardization of an Iron (ii) solution with a standard dichromate solution over Pt & Calomel assembly.
- Determination of purity of Ce (IV) Sulphate with a standard Iron (II) solution over Pt & Calomel assembly.
- Estimation of Iodide with Standard $AgNO_3$ over Pt & Calomel assembly using I^- \ I2 redox couple.
- Simultaneous determinations of Chloride and Iodide ions with Standard $AgNO_3$ over Ag-Glass electrode assembly.
- Determination of the purity of $[Co (NH_3)_5Cl] Cl_2$ over Ag-Glass electrode assembly.
- Complexometric titration for determination of Ferro cyanide with standard Zinc (ii) solution and inorder to establish the composition of the complex $K_2Zn_3[Fe(CN)_6]_2$

E: - pH-metric Titrations: **(2 Experiments)**

- Quantitative analysis of Chromate Dichromate mixture by pH Titration.
- Purity of Acetyl Salicylic acid (Asprin) in a commercial tablet by pH Titration.

F: - Conductometric Titrations: **(2 Experiments)**

- To determine the solubility and solubility product of a sparingly soluble salt ($BaSO_4$) in water.
- To determine the basicity of sodium potassium tartarate by Conductometric method.

G:- Spectrophotometry: **(5 Experiments)**

- Determination of Iron (II) with 1,10-Phenanthroline.
- Determination of Phosphate by Molybdenum blue method.
- Determination of formula of Iron (III) thiocyanate complex by Job's Continuous variation method.
- Determination of composition of Iron (II)—2,2-bipyridyl complex by Mole ratio method.
- Determination of rate of Aquation of complex $[Co(NH_3)_5Cl]Cl_2$ in acidic medium.

H: - Flame Photometry: **(2 Experiments)**

- Simultaneous determination of Sodium and Potassium in the given mixture.
- Determination of Cadmium and Magnesium in tap water.

Books Recommended:

- Vogel's quantitative analysis 6 Edn. Mendham, Denny; Pearson Education 2002
- Synthesis and Technique in Inorganic chemistry , G. S.Girlomi; R.J. Angleci 3rd edn.; University Science Books.
- Synthesis and characterization of Inorganic compounds W.AJolly
- Inorganic syntheses Vols II, VI Academic Press.
- Experimental Inorganic / Physical Chemistry ; Mounir A. Malati Horwood/1999.
- Quantitative Chemical Analysis ; 5th edn.; Harris ; Freeman ; 1999.
- Advanced Practical Inorganic Chemistry ; Adams ; Raynor, Wiley ; 1995.
- Advanced Experimental Inorganic Chemistry ; Ayodha Singh ; Campus Books 2002.

Course No: CH17411DCE
Title: Advanced Laboratory Course in Organic Chemistry (04 Credits)

Max. Marks: *100* — ***Duration:*** *64 Contact hours*
External Exam: *75 Marks.* — ***Internal Assessment****: 25 Marks*

1. **Multistep synthesis of drugs/ organic coinpouiuls involving name reactions**
   (1) Synthesis oflocal 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.
2. **Extraction/Estimation of Organic compounds from Natural sources**
   (1) Isolation of lycopene and β-carotene from tomato and their characterization using *uv*- spectroscopy.
   (2) Isolation of limonene from its natural source and physicochemical analysis.
   (3) Assay of Belladona for Hyoscyamine.
   (4) Assay of lemon from citric acid and vitamin-C
   (5) Isolation of cholesterol from gallstone
   (6) Assay of coke (soft drink)
3. **Column Chromatography**
   Separation of two component solid mixture. Identification of separated components using physical, chemical and spectral techniques.
4. **Spcctrophotomctric estimation** (UV/visible)
   (1) Vitamin-C (Ascorbic acid)
   (2) Caffeine from tea.
   (3) Cholesterol
   (4) Aspirin
5. **Elcctrophoresis/ Paper chromatography**
   Separation and identification of aminoacids by elcctrophoresis / Paper chromatography.
6. **Spcctroscopy**
   Identification of Organic compounds through interpretation of their spectra (UV, IR, PMR, CMR and Mass. Spectra to be provided).

Books Recommended :

1. Comprehensive Practical Organic Chemistry, V.K. Ahluwalia, Renu Aggarwal (Univ. Press India Limited -2000).
2. Vogel's Text Book of Practical Organic Chemistry, B.S.Furniss, A. J. Hannaford (AWL 5th Ed.-1998).
3. Organic Laboratory Techniques , Donald .C. Pavia, Gary . M. Lampman (SCP 3rdEd.-1999)
4. Experiment Organic Chemistry, John.C. Gilbert., Stephen.F.Martin (SCP -1998)
5. Advanced Practical Organic Chemistry Vol. II, Jag Mohan (Himalaya Pub. House First Ed.-1992.

Course No: CH17412DCE
Title: Advanced Laboratory Course in Physical Chemistry (04 Credits)

Max. Marks: *100* — ***Duration:*** *64 Contact hours*
External Exam: *75 Marks.* — ***Internal Assessment****: 25 Marks*

A. Tensiometry

1. Investigation of variation of surface tension of n-butanol and sodium chloride solutions with concentration and hence determination of their surface excess concentrations using Gibb's Adsorption Isotherm.
2. Determination of CMC value of a detergent using tensiometry.

B. Cryoscopy

1. Investigation of variation of freezing point depression with concentration & determination of molecular mass.
2. Determination of the degree of dissociation of a salt/weak acid in solution.
3. Determination of activity co-efficient from freezing point measurements.

C. Spectrophotometry

1. To study the complexation reaction between Fe(III) & salicylic acid.
2. Determination of pK value of an indicator.

D. Spectrofluorometry

1. To determine the rate constant for fluorescence quenching of anthracene or perylene by CCl_4 in ethanol.
2. Using pyrene as probe determine the cmc of a surfactant and site of solubilization of pyrene in the micelle through spectrofluorometry.

E. Potentiometry

1. Precipitation titration of KCl, KBr, KI and their mixture with $AgNO_3$
2. Thermodynamics of a chemical reaction by EMF-method.
3. Determination of (a) Standard electrode potential & (b) Activity Coefficient.

F. Conductometry

1. Verification of Debye-Huckel-Onsagar law.
2. Precipitation titration of $BaCl_2$ and K_2SO_4/ $(NH_4)_2SO_4$
3. Estimation of the concentrations of H_2SO_4, CH_3COOH and $CuSO_4$ in a mixture.

G. Dynamic Electrochemistry

1. To estimate the surface area of a working electrode through chronoamperometry and chronocoulometry.
2. Using Cyclic Voltammetry to determine the formal potential and diffusion coefficient of $[Fe(CN)_6]^{3-}$.
3. Use cyclic voltammetry to determine the concentration of acetaminophen in a given sample.

H. Kinetics

1. Kinetic Investigation of BZ-Oscillatory reaction.
2. Kinetic study of enzyme catalyzed reaction (effect of pH and Temperature).

I. Viscometry and densitometery

1. Determination of Mol. Mass of a Polymer (Polyv inyl alcohol) using viscosity method.
2. To explore the nature of chemical bonding (head-head and Head tail linkage of monomers) in polyvinyl alcohol using Viscometry.
3. Determination of partial molar volume of sodium chloride solutions as a function of concentration from density measurements.

Books Recommended

1. Practical Physical Chemistry --- Findley revised by Kitchner.(Longman, 1971)
2. Experimental Physical Chemistry, A. M. Halpern, G. C. McBane, (Freeman, 2006)
3. Experiments in Physical Chemistry, 5th ed. --- Schoemaker et al. (MGH, 2003)
4. Experimental Electrochemistry---R. Holze (Wiley-VCH, 2009).

Course No: CH17413DCE

Title: Supramolecular Chemistry (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*

Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Supramolecular Interactions (08 Contact hours)

Definition and Development of Supramoleclar Chemistry. Nature of Supramolecular Interactions.

Hard Soft Acid Base Concept- Concept, Classification, Symbiosis. Utility in drug design and molecular recognition. Soft Ligands for Soft Metal Ions-Mixed Crown Ethers and Mixed Cryptands.

Unit-II Supramolecular Receptors (08 Contact hours)

Cation Receptors: Supramolecular Cation Coordination Chemistry, EDTA- The Supramolecular Host. Introductory account of Cation Receptors - Podands, Corands, Cryptands, Spherands and Calixarenes.

Anion Receptors: Scope and Challenges, Anion Hydrophobicity-Hofmeister Series, Introductory Account of Anion Receptors - Cyclophanes, Pyrolles, Azacrowns and Metal Based receptors. Hydride Sponge and Anticrowns.

Ion-Pair Receptors: Concept and Significance

Unit-III Crystal engineering and Supramolecular Motiffs (08 Contact hours)

Crystal Engineering: Introduction, Tectons and Synthons. Hydrogen Bond- Introduction, Criteria

Nature and Importance.

Self Assembly: Scope and Objectives. Concepts and Classification. Introductory Account of Coordination Capsules, Catenenes, Rotaxenes and Molecular Knots.

Unit-IV Network Solids and Molecular Devices (08 Contact hours)

Network Solids: Concepts and Classification, Network Topology. Zeolites: Structure, utility and limitations. Metal Organic Frameworks-Introduction and application in catalysis and Gas storage.

Molecular Devices**:** Philosophy of Molecular Devices, Photophysical Fundamentals and Mechanism of Energy and Electron Transfer, Introductory Account of Molecular Wires, Molecular Switches and Molecular Motors.

Books 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, Ist 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. Chemical Reviews. Vol. 115, Issue 15, year **2015**, Pages 6999-8156
8. Introduction: Supramolecular Chemistry. F. Huang and E. V. Anslyn. Chem. Rev. **2015**, 115, 6999−7000.
9. Supramolecular materials. D. B. Amabilino, D. K. Smith and J. W. Steed. Chem. Soc. Rev., **2017**, 46, 2404—2420
10. A Bond by Other Name. G. R. Desiraju. Angew. Chem. Int. Ed. **2011**, 50, 52-59.
11. The Weak Hydrogen Bond: In Structural Chemistry and Biology. G. Desiraju, T. Steiner. **Oxford, IUCr Monograph on Crystallography**.

Course No: CH17414DCE
Title: Designing Organic Synthesis (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I (A) Oxidative and Reductive Processes in Organic Synthesis (8 Contact hours)

Oxidation**:** Introduction, Aromatisation of cycloalkanes and alkenes using metal catalysts and DDQ. Oxidation of Alcohols using chromic acid, DCC and Swern reagent. Oppenaur oxidation. Oxidation of ketones. Oxidation at activated carbon-hydrogen bond. Oxidation with Selenium dioxide. Prevost hydroxylation and its modification by Woodward.

Reduction**:** lntroduction. Reduction of Alkenes, Alkynes and Aromatic rings.

Reduction of carbonyl compounds: Clemmensen and Wolf-Kishner reductions. Reductions using $LiAlH_4$ and $NaBH_4$ Bouveault-Blanc reduction. Reduction of Epoxides, Nitro, Nitroso, Azo and Oxime groups. Reductions using Tributyl Tin Hydride.

(B) Protection and Interconversion of Functional Groups (8 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-II 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, α, β-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; Verlage VCH;1986.
3. Principles of Organic Synthesis 2nd edn;. R. O. C. Norman; Chapman and Hall; 1978.
4. Advanced Organic Chemistry Part B, 5th edn.; F. A. Carey and R.J Sundberg ; Springer; 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, 6lh Ed., J. March,; Wiley; 2012.
9. Organic Synthesis- The disconnection Approach; Sturat Warren; Wiley; 2013

Course No: CH17415DCE
Title: Computational Chemistry (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I

(a) Numerical solution of equations **(8 Contact hours)**

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

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

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

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

(b) Numerical differentiation and integration **(8 Contact hours)**

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

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

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

Unit-II

(a) Interpolation and Curve Fitting **(8 Contact hours)**

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

Lagrange's interpolation method, Newton's divided differences, Cubic spline, piece wise interpolation.

Least squares approximation, linear and quadratic.

(b) Use of Mathematica/Scilab for numerical solution of problems(8 Contact hours)

The mathematica package will be used for the solution of problems covered under the above three units.

Books Recommended

1. Data Reduction & Error Analysis, Bevington& Robinson, (McGraw-Hill, 2003)
2. Computational Chemistry, A. C. Norris, (Wiley.)
3. Computer Software Applications in Chemistry - P. C. Jurs, (John Wiley, 1996.)
4. Numerical Methods for Scientists and Engineers, H. M. Antie, (TMH,).
5. Numerical Recipes in Fortran/C, W.H. Press et al., (CUP,1992)
6. Applied Numerical Analysis, Gerald &Wheatly, (Pearson Education, 2002)
7. Mathematical Methods for Scientists and Engineers, D.A. McQuarie, Viva Books, 1st Ed., 2009.
8. Mathematica Manual.

Course No: CH17416DCE
Title: Seminar (02 Credits)

Presentation by a candidate on any topic chosen in consultation with the teacher incharge.

(25 Marks)

Manuscript (on the topic) submission (25 Marks)

Course No: CH17417GE
Title: Synthetic Polymers and their Applications (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

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

Course No: CH17418GE
Title: Novel Materials (02 Credits)

Max. Marks: *50* — ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit (Term end) Exam:*** *25 marks*

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

Block Copolymers: Introduction: classification, micellization of diblock 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, photoconductivity and sensors.

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

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

Luminesence and phosphors. Lasers - general principle of lasing action, Ruby laser, semiconducing 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 Nanofluids 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, Jeremy Ramsden and Ventus Publishing ApS, 2009.

Course No: CH17419OE
Title: Food Chemistry (02 Credits)

Max. Marks: *50* — ***Duration:*** *32 Contact hours*

Ist Unit Exam: *25 marks* — ***IInd Unit (Term end) Exam:*** *25 marks*

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_2, 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; 3rd Ed.; Marcel Dekker, Inc. NY; 2005.
2. Food: The Chemistry of its components; T.P. Coultate; 3rd 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; 2nd ed.; Springer International Edition; 2005.

Course No: CH17414DCE
Title: Designing Organic Synthesis (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I (A) Oxidative and Reductive Processes in Organic Synthesis (8 Contact hours)

Oxidation**:** Introduction, Aromatisation of cycloalkanes and alkenes using metal catalysts and DDQ. Oxidation of Alcohols using chromic acid, DCC and Swern reagent. Oppenaur oxidation. Oxidation of ketones. Oxidation at activated carbon-hydrogen bond. Oxidation with Selenium dioxide. Prevost hydroxylation and its modification by Woodward.

Reduction**:** lntroduction. Reduction of Alkenes, Alkynes and Aromatic rings.

Reduction of carbonyl compounds: Clemmensen and Wolf-Kishner reductions. Reductions using $LiAlH_4$ and $NaBH_4$ Bouveault-Blanc reduction. Reduction of Epoxides, Nitro, Nitroso, Azo and Oxime groups. Reductions using Tributyl Tin Hydride.

(B) Protection and Interconversion of Functional Groups (8 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-II 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, α, β-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).

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1. Designing Organic Synthesis, S. Warren ;Wiley; 2013.
2. Organic Synthesis- concept, methods and Starting Materials, J. Furhop and G. Penzlin; Verlage VCH;1986.
3. Principles of Organic Synthesis 2nd edn;. R. O. C. Norman; Chapman and Hall; 1978.
4. Advanced Organic Chemistry Part B, 5th edn.; F. A. Carey and R.J Sundberg ; Springer; 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, 6lh Ed., J. March,; Wiley; 2012.
9. Organic Synthesis- The disconnection Approach; Sturat Warren; Wiley; 2013

Course No: CH17401CR
Title: Organo-Transition Metal Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Sigma Bonded Organometallic Compounds: (16 Contact hours)

Classification, Stability, Comparison to main Organometallic Compounds, Routes of synthesis, Reactions. Decomposition Pathways: Choice, α and β hydrogen transfer. Intramolecular elimination of alkane, Cyclometallation, Stability from bulky substituents, Agostic alkyls, Umpolung.Metal Hydride Complexes: Synthesis, Characterization and Chemical reactions, Non-classical Hydrides (Kubas complexes).

Unit-II Pi-bonded Organometallic Compounds: (16 Contact hours)

Classification, Structure and bonding in Metal- alkene, alkyne, allyl, 1,3-butadiene and Cyclobutadiene Complexes.

Sandwich Compounds: Characteristics; Classification, Synthesis, Reactions, 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.

Unit-III Catalytic Processes involving Transition Metal Organometallic Compounds: (16 Contact hours)

Mechanistic aspects: Oxidative addition, Insertion reactions Reductive elimination and water gas shift reaction (WGSR).

Catalytic mechanism of Hydrogenation, Hydroformylation, Oxidation and Isomerization of alkenes; Olefin metathesis.

Fischer-Tropsch Synthesis and Ziegler Natta polymerization of alkenes.

Asymmeteric and supported Organometallic Catalysis (brief idea)

Unit-IV Fluxional Organometallic Compounds and Synthetic Reactions involving Organo- metallics (16 Contact hours)

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 η^1 Cyclopentadienyls and η^3–allyls.

Stereochemical non rigidity in case of coordination numbers- 4 & 5 (cis-trans, atomic inversion, Berry Pseudorotation).

Synthetic Reactions involving Organo- metallics:

Reactions of coordinated ligands, carbon monoxide, alkyls, alkenes (Green, Mingo's rules). Activation of small molecules: Carbon monoxide, Carbon dioxide and Alkanes.

Role of organo-iron as synthons, Carbon-Carbon coupling and its reactions (Suzuki and Heck).

Books Recommended:

1. The Organometallic Chemistry of Transition Metals; 2nd edn; Robert. H . Crabtree; Wiley; 1994.
2. Fundamental Transition Metal Organometallic Chemistry; Luke hart; Brooks / Cole; 1985.
3. Organometallic Chemistry; 2nd edn ; Mehrotra & Singh ; New age international 2000
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 press 1983.
9. Reaction Mechanism of Inorganic and Organometallic systems; 2nd edn.; Robert .b. Jordan 1998.
10. Inorganic Chemistry ; 4th edn.; Huheey ; E. Keiter & R. Keiter; Addison-Wesley ;1983
11. Modern Inorganic Chemistry; William. A. Jolly; McGraw Hill; 1985.

Course No: CH17402CR
Title: Photo-Inorganic Chemistry (04 Credits)

Max. Marks: *100* — ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Basics of Photo-Chemistry (16 Contact hours)

Absorption; mechanism of absorption of light

Transition moment integral, Einstein's treatment, molar integrated absorption intensity, natural radiative lifetime & the calculation of life times.

Excitation; d-d transition, charge transfer & intraligand 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 diagramsdepicting excited states.

Frank Condon principle, shapes of absorption & emission bands.

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

Tools and Technique: Light source, measurement of light intensity, chemical actinometry. Flash photolysis.

Unit-II The Chemistry of Excited State Molecules (16 Contact hours)

Photochemical laws & quantum yield. Kinetics & quantum yield of photo-physical (radiative) and photo-chemical processes. Photochemical processes: primary, secondary, adiabatic & non- adiabatic. Properties of thexi states; Determination of dipole moments & acidity constants of excited state molecules.

Photosubstitution and photo reduction of Co (III) complexes.Photosubstitution reaction of Cr (III) and Rh (III) complexes.

Organometallic-Photochemistry: Reactions of metal carbonyls, cleavage of metal-metal bond.

Unit-III Redox Reactions by Excited Metal Complexes (16 Contact hours)

Energy transfer under conditions of weak and strong interaction. Excited state electron transfer. Marcus-Hush model.Conditions of the excited states to be useful as redox reactants. Photochemical electron transfer, [Ru (bipy)3]2+ and [Os (bipy)3]2+.

Photochemical supramolecular devices: devices for photo-induced energy or electron transfer, Devices for information processing, photo-chemically driven molecular machines.

Unit-IV Solar Energy-Prospects and Challenges (16 Contact hours)

Solar energy storage, solar energy conversion, Metal complex sensitizers and electron relays in photochemical splitting of water, Nitrogen fixation and CO_2 reduction. Inorganic photolithography.

Supramolecular photochemistry in natural systems: photosynthesis, bacterial photosynthesis and artificial photosynthesis.

Books Recommended:

1. Reaction Mechanisms of Inorganic and Organometallic Systems; 2nd edn.; Jordon; Oxford; 1998.
2. Mechanism of Inorganic Reactions; Katakis, Gordon; Wiley; 1987.
3. Inorganic Chemistry; 4* edn; Huheey; Harper & Row; 1990.
4. Mechanism of Inorganic Reactions, 2nd edn, Basalo, Pearson; Wiley Eastern, 1997.
5. Chemistry of Light; Suppan, Royal Society; 1994.
6. Photochemistry, Carol J. Wayne and Richard P. Wayne; Oxford University Press; 1996.
7. Fundamentals of Photochemistry; C Rohatgi, Mukhergi; Wiley Eastern.; 1992
8. Inorganic Photochemistry; J.Chem Edu.;Vol .60, No.10,1983.
9. Applications of Inorganic Photochemistry; J. Chem. Edu.; Vol.74, No 69. 1997.

Course No: CH17403CR
Title: Bio-Inorganic Chemistry (04 Credits)

Max. Marks: *100* — ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Iron Storage, Transport and Oxygen carriers: (16 Contact hours)

Structure and Coordinating sites in biologically important ligands: Proteins, Nucleotides and Lipids.

The transport mechanism: uniport, symport and antiport.

Ferritin and Transferrin: Structure, Metal binding sites; incorporation and release of iron.

Porphyrins: Introduction, characteristic absorption spectrum and salient characteristics.

Haemoglobin and Myoglobin: Structure, oxygen saturation curves; Mechanism of oxygen transport and storage.Bohr effect and cooperativity in haemoglobin.

Hemerythrin and Hemocyanin: Structure, Metal binding groups and Dioxygen binding. Synthetic oxygen carrier model compounds: Vaska's iridium complex: Cobalt complexes with micro and macrocyclic ligands and Schiff base ligands.

Unit-II Metallo-enzymes and Electron Carriers (16 Contact hours)

Enzyme, Apoenzyme, Coenzyme, Prosthetic group and Metalloenzymes, Mechanism of enzyme action.

Zinc enzymes:- Carboxypeptadiase and Carbonic Anhydrase : Introduction, Structure, Mechanism of action and their model compounds.

Biological chemistry of Molybednum: uptake of Molybednum; oxidation states and redox potentials in enzymes and oxygen atom transfer reactions.

Xanthine oxidase and Aldehyde oxidase: Structure and biological role.

Cobalt in Vitamin B_{12}: Introduction, Structure and Derivatives of B_{12} and mechanism of alkylation reaction. Role of vitamin B_{12}.

Electron Carriers: Rubredoxin & Ferridoxin (Structure and biological role).

Blue Copper proteins: Oxidases and Plastocyanin (Structure and biological role).

Unit-III Metal-ion Induced Toxicity and Chelation Therapy (16 Contact hours)

Toxic levels of different metals. Sources of metal ion poisoning (external sources and internal disorders).

Mechanism of metal ion induced toxicity:- Toxicity of Pb, Cd, Hg, As, and CN- Metal ion promoted Carcinogenesis and probable mechanism of action.

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 Metal Salts and Metal Complexes in Therapeutics (16 Contact hours)

Treatment of essential metal deficiencies: Iron, Copper and Cobalt.Metal salts as anti-acids, antiseptic and diuretics.

Gold compounds and Rhematoid arthiritis.

Anti-Cancer Drugs: cis-Platin and its derivatives. Structure-function relationship.

Complexes of Rhodium, Gold and Cobalt.

Anti-bacterial, Anti-viral and Anti-fungal activities of Metal Complexes: Labile and Robust metal complexes; Probable mechanism of action.

Books Recommended:

1. As listed for Course No. CHM—101 (Inorganic chemistry-M.Sc. 1st Semester! From serial No. 1 to 5.
2. Bio inorganic Chemistry -An introduction; Ochai, Allyn and Bacon; 1977.
3. Inorganic Bio-chemistry—Vol. 1&2; Eichhorn; Elsevier, 1973.
4. Inorganic Aspects of Biological and Organic Chemistry; Hanzilik; Academic; 1976.
5. The Inorganic Chemistry of Biological processes; 2nd edn.; Hughes ; Wiley; 1973.
6. A Text book of Medicinal aspects of Bio inorganic Chemistry; Das; CBS; 1990.
7. The Biological Chemistry of Elements; Frausto de Silva; Williams; Clarenden; 1991.
8. Principles of Bio inorganic Chemistry; Lippard, Berg; Univ. Science Books; 1994.
9. Inorganic Chemistry in Biology; Wilkins C & Wilkins G; Oxford; 1997.
10. Bio inorganic Chemistry ; K. Hussain Reddy; New Age International (P) Ltd; 2005.
11. Metal -Ions in Biochemistry; P. K. Bhattacharya; Narosa Publishing House; 2005.

Course No: CH17404CR
Title: Heterocyclic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Structure and Nomenclature of Heterocyclic compounds (16 Contact hours)

Introduction and significance of heterocycles in day to day life.

Nomenclature of Heterocycles: Monocyclic, bicyclic and polycyclic heterocycles, Hantzsch-Widman and replacement methods of nomenclature.

Structural features: Non-aromatic, aromatic and heteroaeromatic heterocycles.

Tautomerism in heterocycles, Meso-ionic systems.

Spectroscopic properties of heterocycles (UV,Visible and ^{1}HNMR).

Unit-II General Approach to Synthesis of Heterocyclic compounds (16 Contact hours)

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 quinoline, Bischler-Napieralki Isoquinoline,Knorr Pyrrole,Paal-Knorr , Fischer – Indole synthesis.

Unit-III Monocyclic Heterocycles (16 Contact hours)

Structure, Synthesis and Reactions of Oxirane, Thirane, Azetidine, Pyrrole, Furan, Thiophene, Diazenes, Pyrimidines,Pyridine.Chemistry of five membered heterocycles with two heteroatoms like 1,3-Azoles, 1,2- Azoles. Chemistry of Six membered rings like Azines and seven membered heterocycles like Azepine,Oxipene,Thiepins.

Unit-IV Bicyclic Heterocycles (16 Contact hours)

Structure, Synthesis and reactions of Benzo- fused heterocycles like Benzo-pyrrole, Benzo-furan,Benzo-thiophene, Quinoline, Isoquinoline, Chromones, Coumarins, Iso-Coumarins, 2 and 4-benzopyrones, Benzopyryllium salts and purines.

Books Recommended:

1. Heterocyclic Chemistry, 5th Ed. J.A.Joule and K.Mills, (Wiley-2010).
2. Essentials of Organic Chemistry, Paul M Dewick , (Wiley-2006).
3. Heterocyclic Chemistry, J.A. Joule and G.F.Smith , (Chapman and Hall-1996).
4. The Chemistry of Heterocycles Theophil Eicher and Siegfried Hauptmann , (George Thieme Verlag Stutt gart,New York -1995).
5. Heterocyclic Chemistry, Raj K. Bansal, (New Age International Publisher-2006).
6. Heterocyclic Chemistry, R.R.Gupta,M.Kumar,V.Gupta,(Springer-2006).

Course No: CH17405CR
Title: Chemistry of Natural Products (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Terpenoids and Carotenoids (16 Contact hours)

Introduction, classification, general methods of isolation, separation.

Essential oils: Separation using Gas Liquid Chromatography and High Performance Liquid Chromatography. Physical, chemical and spectral methods of structure elucidation.

Structure determination, stereochemistry and synthesis of α-terpineol, abietic acid and β-carotene.

Unit-II Alkaloids (16 Contact hours)

Introduction, classification, nomenclature, qualitative tests, pharmaceutical applications and general methods of isolation. Physical, Chemical & Spectral methods of structure elucidation.

Stereochemistry, synthesis and biosynthesis of Quinine, Morphine and Reserpine.

Unit-III Steroids (16 Contact hours)

Introduction, nomenclature, classification & stereochemistry. Physical, Chemical & Spectral methods of characterization. Qualitative tests.

Cholesterol: Isolation, clinical significance, chemical properties, structure elucidation, total synthesis & relationship with bile acids.

Sex hormones: Introduction, isolation, clinical & commercial significance, color reactions, structure determination and partial synthesis of Oesterone, Androsterone, Testosterone and Progesterone.

Glucocorticoids & Mineral Corticoids: Introduction and partial synthesis of Cortisone, aldosterone and synthesis of cholecalciferol.

Unit-IV Natural Plant Pigments and Porphyrins (16 Contact hours)

Introduction, classification, physical, chemical, degradative and spectral methods of structure determination and biosynthesis (Acetate and Shikimic acid pathway)

Flavonoids: Isolation, separation and quantification. Antioxidant activity of flavonoids. Robinson's synthesis, Baker Venketraman synthesis, Kostanecki synthesis of flavanone and Flavanol.

Isolation, structure determination and synthesis of Cyanidin, Chrysin, Quercitin & Genestein.

Porphyrins: Structure determination and total synthesis of haemoglobin. Structural comparison with chlorophyll.

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. New Trends in Natural Product Chemistry, Atta-ur-Rahman (Harward Academic Press).
4. Chemistry of Natural Products, N.R. Krishnaswamy (University Press-1999).
5. Flavanoids; Oyvind M. Andersen and Kenneth R. Markhan. (Taylor & Francis -2006)

Course No: CH17406CR
Title: Bio-Organic and Medicinal Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I (16 Contact hours)

Vitamins:_ Source, structure and synthesis of vitamins – Vitamin A, Vitamin B-Complex (Thiamine riboflavin, folic acid); Vitamin B-12 (Structure only) Vitamin C, E, K, H and D.

Prostaglandins : Introduction and nomenclature, approaches to prostaglandin synthesis, cyclo-hexane, precursors-Woodward synthesis of PGF2a. Cyclo-heptane precursors - Corey's synthesis of prostoglandin's E & F.Their relationship with oxygenase I and II.

Nucleic Acids: Structure of nucleotide, nucleosides, RNA and DNA, role of nucleic acids in protein synthesis, genetic code and heredity. DNA finger printing

Unit-II (16 Contact hours)

Enzymes : Introduction, nomenclature & classification.. Activation & inhibhion of enzymes. Mechanism of enzyme action- Fischer lock and key, koshlands induced fit hypothesis, displacement reactions & coupling of ATP. Enzyme mechanism of chymotrypsin lysozyme & carboxypeptidase.

Co-Enzymes: Cofactors derived from vitamins, coenzymes, prosthetic groups. Apoenzyme. Structure , biological function and mechanism of reactions catalsed by co-enzymes: coenzyme A, thiamine pyrophosphate. pyridoxal phosphate, NAD+, NADP+, FMN, FAD and Lipoic acid.

Unit-III (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, carbonylic, thiols sulphides groups and introdction/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. Lipophillic constant, Hamett constant, steric parameters and Hansch analysis.

Unit-IV (16 Contact hours)

Antibiotics: Classifications-structural and mechanistic, cell wall biosynthesis inhibitors, protein synthesis inhibitors. Pencillins-classification and structures. Synthesis of Pencillins, V, G, chloroamphenicol.and ciprofloxacin. Tetracyclins.

Psychoactive Drugs: Introduction, CNS depressants, CNS stimulants, sedatives and hypnotics, barbutirates. Synthesis of diazepam, phenytoins and glutethisimide.

Anti-neoplastic drug: Introduction; cancer chemotherapy, carcenoolytic antibiotic, plant derived anti-cancer agents (Taxol)role of alkylative agents and antimetabolites in treatment of cancer, mitotic inhibitors (elementary idea).

Cardiovascular Drugs: Introduction, cardiovascular diseases, synthesis of Amylnitrate. sorbitrate, quinidine, verapanil, methyl dopa and atenolol

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, Biotechonolgy and Clinical Chemistry of Enzmyes. Trevor Palmer (EWP)
5. Organic Chemistry by I.L.Finar Vol. II (ELBS Longamnn)
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. Chemsitry of Natural Products. S.V. Bhat, B.A. Nagasampagi, M. Siva Kumar. Naroosa Publishing House, New Delhi.

Course No: CH17407CR
Title: Advanced Quantum Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Electronic Structure Theory, Hartree-Fock Method (16 Contact hours)

Review: Electronic Hamiltonian, antisymmetrized wave function, Slater determinant. Hartree-Fock self-consistent field method. One and two-electron integrals in the light of minimal basis H_2 system.

Hartree-Fock Equation, Fock, Coulomb and exchange operators and integrals, restricted Hartree-Fock formalism, Roothaan equation. The Fock matrix elements, Koopman's theorem, Slater-Condon rules. Matrix form of Roothaan equation, the SCF procedure.

Basis Sets: Slatter-type orbitals, Gaussian basis sets. Model SCF calculations on H_2 /$HeH^{+.}$

Unit-II Configuration Interaction and Semiempirical methods (16 Contact hours)

Configuration Interaction: Electron correlation, configuration state functions, configuration interaction (CI), Brillouin theorem, full and truncated CI theories- CID, CISD, CISDTQ methods; Size consistency problem. Moller-Plesset and Coupled Cluster methods.

Semiempirical methods: The ZDO approximation; the PPP method, brief idea of CNDO, INDO and NDDO methods. The MINDO, MNDO, AM1 and PM3 methods.

Unit-III Density Functional Methods and Molecular Properties (16 Contact hours)

Density Functional Theory:Electron probability density. Hohenberg-Kohn theorems, Kohn-Sham formulation of DFT, n- and v- representabilities, E_x&$E_c$functionals; the local density and local spin density approximations, gradient corrected and hybridfunctionals.
Brief idea of Molecular mechanics methods, force fields.

Molecular Properties*:* Potential energy surfaces; molecular geometry and its optimization, Hessian Matrix and normal modes, vibrational frequencies, thermodynamic properties. Dipole moments, atomic Charges.

Unit-IV Use of Quantum Chemistry Software: Gaussian (16 Contact hours)

A quick tour of GAUSSIAN Interface. Input to Gaussian. Model calculations illustrating various features of the package**.**

1. A single point energy calculation: HCHO /CH3.CHO,HCHOMOs.
2. Geometry Optimization: Input and Output for ethene, fluoroethene, propene conformers
3. Transition state optimization $CH_2O \rightarrow HCOH$
4. NMR properties of ethane, ethene and ethyne.
5. Frequency Calculations: Input, Formaldehyde frequencies, Normal modes, zero point energy, thermodynamic properties, polarizability, hyperpolarazability.
6. Stationary points characterization –C3H5F
7. Model Chemistries: Basis set effect on HF bond length

8. Selecting an appropriate theoretical method:
   a) Electron correlation and post SCF methods, limitations of Hartree-Fock theory: HF bond energy, Optimization of O_3.
   b) Density Functional Theory: CO_2 structure and atomization energy.
   c) Butane / Isobutane isomerization energy, rotational barrier in n-butane.

9. Chemical reactions and reactivity:
   a) Hydration enthalpy of the reaction $H^+ + H_2O \rightarrow H_3O^+$
   b) Potential energy surfaces. Reaction path following (IRC calculation)
   $CH_2O \rightarrow HCOH$
   c) Heat of formation of CO_2 via an isodesmic reaction
10. Solvation models: Formaldehyde Frequencies in Acetonitrile

Books Recommended

1. Quantum Chemistry, Ira. N. Levine, (Prentice Hall, 2009).
2. Quantum Chemistry, 2nd Edn , D. A. McQuarrie, (University Science Books, 2007).
3. Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedmann, (Oxford, 2008).
4. Quantum Chemistry and spectroscopy, Engel & Reid, Pearson (2007)
5. Modern Quantum Chemistry - Introduction to Advanced electronic structure theory - A. Szabo & N. S. Ostlund, (Macmillan, 1982, Dover 1996).
6. Molecular Modeling, Principles and Applications, A. R. Leach, Prentice-Hall, 2001
7. Modern Electronic Structure Theory, D. R. Yarkouy (ed). (World Scientific, 1995)
8. Ab Initio Molecular Orbital Theory, by Hehre, Radom, Schleyer and Pople, (Wiley)
9. Density Functional Theory of Atoms and Molecules, R.G. Parr and W. Yang, Oxford(1989).
10. GAUSSIAN Manual, Gaussian Inc
11. Exploring chemistry with electronic structure methods, Foresman J.B., Frisch A., Gaussian Inc

Course No: CH17408CR
Title: Advanced Electrochemistry and Statistical Mechanics (04 Credits)

Max. Marks: *100* — ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Instrumental Methods in Electrochemistry (16 Contact hours)

Fundamentals: Electrode potential and its measurement, standard and formal electrode potentials, three electrode measurements, uncompensated resistance.

Overview of electrode Processes: Faradaic and Non-Faradaic processes, factors affecting electrode reaction rate. Mass transfer: Convection, migration, diffusion, Fick's 1st and 2^{nd} law of diffusion,

Electrochemical Techniques:

Electrophoresis: Factors affecting ion migration, electro-osmosis, theory and applications of capillary electrophoresis.

Potential Step Methods: Chronoamperometry, Chronocoulometry at macro electrodes; theory and applications. Cottrell equation. Controlled-Potential coulometry, Constant-Current coulometric titrations.

Potential Sweep Methods: Linear sweep Voltammetry and Cyclic Voltammetry at macro electrodes theory and applications, Diagnostic criteria of Cyclic Voltammetry.

Unit-II Applied Electrochemistry (16Contacthours)

Electrochemistry of redox enzymes: Direct and mediated electron transfer, Enzyme modified electrodes-challenges and applications. Mechanism and approach to bioelectrosynthesis, examples of bioelectro synthesis-oxidation of alcohols, synthesis of dihydroxy acetone phosphate, site specific oxidation of sugars, reduction of carbonyl compounds, hydrogenation.

Energy storage devices: Desirable characteristics of energy storage devices, Discharge plot, Ragone plot. Batteries: Measures of battery performance. Classical batteries (Lead Acid, Nickel-Cadmium, Zinc-Mangenese dioxide). Modern batteries (Zinc-Air, Nickel-Metal Hydride, Lithium Ion Batteries), Supercapacitors.

Fuel cells, types of fuel Cells, basic fuel cell operation, kinetics of fuel cell reactions. Alkaline, Phosphoric acid, Polymer Electrolyte membrane and direct MeOH fuel cell, biofuel cells.

Unit-III Classical Statistical Mechanics and Ensemble concept (16 Contact hours)

Equations of Motion; Newton, Lagrange and Hamiltonian. Classical partition function, phase space and the Liouville equation, Kinetic theory of gases, equi-partition of energy, Maxwell's velocity distribution.

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. Statistical Mechanical treatment of imperfect gases. Virial equation of state from grand

partition function, virial coefficients in the classical limit, second and third virial coefficients.

Unit-IV Applied Statistical Mechanics (16 Contact hours)

Quantum Statistics: Fermi-Dirac and Boson-Einstein statistics, Nuclear spin statistics, symmetry and nuclear spin, Ortho and Para nuclear spin states, Ortho and Para Hydrogen and Deuterium, CO.

Application of grand partition function to Boson-Einstein and Fermi-Dirac statistics. Ideal Fermi-Dirac gas: Electrons in metals, Ideal Photon gas: Black body radiation, influence of wavelength for the Planck distribution, Bose-Einstein condensation.

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. Electrochemical Methods Fundamentals and Applications, 2ndEdition, Allen J.Bard, Larry R. Faulkner, John Wiley and Sons, INC.
2. Physical Electrochemistry-Principles, Methods and Applications, Israel Rubinstein (Ed.) Marcel Dekker, Inc. New York.
3. Understanding Voltammetry, 2nd Edition, Imperial College Press.
4. Elements of Molecular and Biomolecular Electrochemistry, Jean-Michel Saveant, Wiley-Interscience.
5. Electrochemistry, 2nd Edition, Carl H. Hamann, Andrew Hammett, Wolf Vielstich,Wiley-VCH.
6. Modern Electrochemistry 2B, 2nd Edition, J. O`M. Bockris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.
7. Statistical Thermodynamics, M. C.Gupta ,(NewAgeInternational,1993).
8. Statistical Thermodynamics-Fundamentals and Applications, N.M. Laurendeau, Cambridge University Press, 2005.
9. Statistical Mechanics, D.A. McQuarrie, (Viva,2003).
10. Introduction to Statistical Thermodynamics, Chandler, (OUP, 1987).
11. Statistical Thermodynamics and Kinetic Theory, C. E. Hecht, (Dover,1990).
12. Statistical Mechanics –Principles and Applications, Hill, Dover, 1987.
13. Statistical Thermodynamics for Chemists, A. Ben-Naim, (Plenum, 1992).
14. An introduction to Statistical Thermodynamics, Hill, (Addison-wesley,1987).

Course No: CH17409CR
Title: Chemistry of Materials (04 Credits)

Max. Marks: *100* | ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Surfactant mixtures, Stimuli responsive surfactants and block copolymers (16 Contact hours)

Surfactant-Surfactant Interactions: Mixed micelle formation, mixed monolayer formation, synergism, Clint and Rubingh's models of mixed micelle formation**.** Importance and practical applications of mixed surfactant systems.

Stimuli-Responsive Surfactants: Introduction and applications: Biosurfactants, redox, photochromic, thermoreversible, pH-sensitive, cleavable and magnetic surfactants.

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

Unit-II Hydrogels and microemulsions (16 Contact hours)

Hydrogels: Introduction, Types of Hydrogels, Preparation, Properties and characterization of Hydrogels, Biomedical applications of Hydrogels.

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

Unit-III Langmuir Blodgett Films, Liquid crystals and Fullerenes (16 Contact hours)

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.

Fullerenes: Fullerenes- History, bonding, properties, doped fullerenes, fullerenes as superconductors and fullerene related compounds (carbon nanotubes).

Unit-IV Optical materials and Ionic conductors (16 Contact hours)

Optical materials: Luminesence and phosphors. Lasers – general principle of lasing action, Ruby laser, Neodymium-YAG lasers, semiconducing lasers and quantum dot lasers. Nonlinear optical effects, second and third order harmonic generation, nonlinear optical materials.

Ionic Conductors: Introduction to ionic conduction and mechanism. Types of ionic conductors, mechanism of ionic conduction, interstitial jumps (Frenkel); vacancy

mechanism. Super-ionic conductors: Diffusion and transition superionic conductors and mechanism of conduction in superionic conductors; examples and applications of ionic conductors.

Books Recommended:

1. M. J. Rosen, J. T. Kunjappu, “Surfactants and Interfacial Phenomena”, John Wiley & Sons, New York, 4^{th} Edition, 2012.
2. R. D. Vold and M. J. Vold, “Colloid and Interface Chemistry”, Addison-wesley, 1982.
3. .D. Y. Meyer, “Surfaces, Interfaces and Colloid”, VCH Publishers, Inc. 1991.
4. Jonsson, Lindmann, Homberg and Kronberg, “Surfactants and polymers in aqueous solution”, John Wiley and sons, 1998.
5. D. Fennell Evans, H. Wennerstrom, “The Colloidal Domain where physics, chemistry, biology and technology meet” VCH, New York, 1994.
6. Robert J. Hunter, “Foundations of Colloid Science”, Oxford University Press, New York, 2007.
7. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
8. I. W. Hamley, The Physics of Block Copolymers (Oxford University Press, Oxford, 1998.
9. N. Hadijichristidis, S. Pispas and G. A. Floudas Block Copolymers (Wiley, New York, 2003).
10. Introduction to Solids, Azaroff, Tata McGraw,1993.
11. SolidState Chemistry and its Applications, West, Wiley,1989.
12. The Physical Chemistry of Solids, Borg, Biens, Academic press, 1992.
13. Solid State Physics, N. W. Ashcroft and N. D. Mermin, Saunders college, 2001
14. Principles of Solid State, H. V. Keer, Wiley Eastern.
15. The Physics and Chemistry of materials, J.I. Gersten, F.W. Smith, John Wiley and sons, Inc. 2001.
16. Microemulsions: Background, New Concepts, Applications, Perspectives, C. Stubenrauch, Blackwell Publishing Ltd, 2009.
17. M. Sirousazar, M. Foroug, K. Farhad, Y. Shaabani and R. Molaei, Hydrogels: Properties, Preparation, Characterization and Biomedical, Applications in Tissue Engineering, Drug, Delivery and Wound Care, IN Advanced Healthcare Materials, Wiley online Library, 2014.

Course No: CH17410DCE
Title: Advanced Laboratory Course in Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *75 Marks.* ***Internal Assessment****: 25 Marks*

A: - Inorganic Preparations: (5 Experiments)

- Preparation of tetraamminecarbonatocobalt (III) nitrate and its conversion to pentaamminecholorocobalt (III) chloride.
- Preparation of trans dicholoro bis (ethylenediamine) cobalt (III) chloride and its conversion to cis-isomer.
- Preparation of tris (ethylenediamine) nickel (II) chloride dihydrate and its conversion to bis (ethylenediamine) nickel (II) chloride.
- Preparation of bis (acetylacetonato) copper (II) dihydrate.
- Preparation of pentaamminecholorocobalt (III) chloride and study of Linkage isomers by its conversion to pentaamminenitritocobalt (III) chloride and to nitro isomer followed by IR Characterization.

B:- Total analysis of a Coordination compound for determination of various components present.

(1- Experiment)

C: - Separation by Column Chromatography and Estimations: (5 Experiments)

- Separation of Permanganate and Bichromate ions on Alumina column and their Estimation from Beer Law plots.
- Determination of lonisable chloride in a Complex by cation exchange column (separation followed by Mohr's titration of elute for estimation).
- Separation of Cobalt (II) and Nickel (II) on anion exchange column followed by estimation through EDTA titrations.
- Separation of two Cobalt (III) complexes viz $[Co(NH_3)_6] Cl_3$ and $[Co (NH_3)_5 Cl] Cl_2$ on Silica column.
- Ion exchange separation of Hydration / ionization isomers of Chromium (III) Chloride ($CrCl_3$).

D: - Potentiometric Titrations: (6 Experiments)

- Standardization of an Iron (ii) solution with a standard dichromate solution over Pt & Calomel assembly.
- Determination of purity of Ce (IV) Sulphate with a standard Iron (II) solution over Pt & Calomel assembly.
- Estimation of Iodide with Standard $AgNO_3$ over Pt & Calomel assembly using I^- \ I2 redox couple.
- Simultaneous determinations of Chloride and Iodide ions with Standard $AgNO_3$ over Ag-Glass electrode assembly.
- Determination of the purity of $[Co (NH_3)_5Cl] Cl_2$ over Ag-Glass electrode assembly.
- Complexometric titration for determination of Ferro cyanide with standard Zinc (ii) solution and inorder to establish the composition of the complex $K_2Zn_3[Fe(CN)_6]_2$

E: - pH-metric Titrations: (2 Experiments)

- Quantitative analysis of Chromate Dichromate mixture by pH Titration.
- Purity of Acetyl Salicylic acid (Asprin) in a commercial tablet by pH Titration.

F: - Conductometric Titrations: (2 Experiments)

- To determine the solubility and solubility product of a sparingly soluble salt ($BaSO_4$) in water.
- To determine the basicity of sodium potassium tartarate by Conductometric method.

G:- Spectrophotometry: (5 Experiments)

- Determination of Iron (II) with 1,10-Phenanthroline.
- Determination of Phosphate by Molybdenum blue method.
- Determination of formula of Iron (III) thiocyanate complex by Job's Continuous variation method.
- Determination of composition of Iron (II)—2,2-bipyridyl complex by Mole ratio method.
- Determination of rate of Aquation of complex $[Co(NH_3)_5Cl]Cl_2$ in acidic medium.

H: - Flame Photometry: (2 Experiments)

- Simultaneous determination of Sodium and Potassium in the given mixture.
- Determination of Cadmium and Magnesium in tap water.

Books Recommended:

- Vogel's quantitative analysis 6 Edn. Mendham, Denny; Pearson Education 2002
- Synthesis and Technique in Inorganic chemistry , G. S.Girlomi; R.J. Angleci 3rd edn.; University Science Books.
- Synthesis and characterization of Inorganic compounds W.AJolly
- Inorganic syntheses Vols II, VI Academic Press.
- Experimental Inorganic / Physical Chemistry ; Mounir A. Malati Horwood/1999.
- Quantitative Chemical Analysis ; 5th edn.; Harris ; Freeman ; 1999.
- Advanced Practical Inorganic Chemistry ; Adams ; Raynor, Wiley ; 1995.
- Advanced Experimental Inorganic Chemistry ; Ayodha Singh ; Campus Books 2002.

Course No: CH17411DCE

Title: Advanced Laboratory Course in Organic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *75 Marks.* ***Internal Assessment****: 25 Marks*

1. **Multistep synthesis of drugs/ organic coinpouiuls involving name reactions**
   (1) Synthesis oflocal 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.
2. **Extraction/Estimation of Organic compounds from Natural sources**
   (1) Isolation of lycopene and β-carotene from tomato and their characterization using *uv*- spectroscopy.
   (2) Isolation of limonene from its natural source and physicochemical analysis.
   (3) Assay of Belladona for Hyoscyamine.
   (4) Assay of lemon from citric acid and vitamin-C
   (5) Isolation of cholesterol from gallstone
   (6) Assay of coke (soft drink)
3. **Column Chromatography**
   Separation of two component solid mixture. Identification of separated components using physical, chemical and spectral techniques.
4. **Spcctrophotomctric estimation** (UV/visible)
   (1) Vitamin-C (Ascorbic acid)
   (2) Caffeine from tea.
   (3) Cholesterol
   (4) Aspirin
5. **Elcctrophoresis/ Paper chromatography**
   Separation and identification of aminoacids by elcctrophoresis / Paper chromatography.
6. **Spcctroscopy**
   Identification of Organic compounds through interpretation of their spectra (UV, IR, PMR, CMR and Mass. Spectra to be provided).

Books Recommended :

1. Comprehensive Practical Organic Chemistry, V.K. Ahluwalia, Renu Aggarwal (Univ. Press India Limited -2000).
2. Vogel's Text Book of Practical Organic Chemistry, B.S.Furniss, A. J. Hannaford (AWL 5th Ed.-1998).
3. Organic Laboratory Techniques , Donald .C. Pavia, Gary . M. Lampman (SCP 3rdEd.-1999)
4. Experiment Organic Chemistry, John.C. Gilbert., Stephen.F.Martin (SCP -1998)
5. Advanced Practical Organic Chemistry Vol. II, Jag Mohan (Himalaya Pub. House First Ed.-1992.

Course No: CH17412DCE
Title: Advanced Laboratory Course in Physical Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *75 Marks.* ***Internal Assessment****: 25 Marks*

A. Tensiometry

1. Investigation of variation of surface tension of n-butanol and sodium chloride solutions with concentration and hence determination of their surface excess concentrations using Gibb's Adsorption Isotherm.
2. Determination of CMC value of a detergent using tensiometry.

B. Cryoscopy

1. Investigation of variation of freezing point depression with concentration & determination of molecular mass.
2. Determination of the degree of dissociation of a salt/weak acid in solution.
3. Determination of activity co-efficient from freezing point measurements.

C. Spectrophotometry

1. To study the complexation reaction between Fe(III) & salicylic acid.
2. Determination of pK value of an indicator.

D. Spectrofluorometry

1. To determine the rate constant for fluorescence quenching of anthracene or perylene by CCl_4 in ethanol.
2. Using pyrene as probe determine the cmc of a surfactant and site of solubilization of pyrene in the micelle through spectrofluorometry.

E. Potentiometry

1. Precipitation titration of KCl, KBr, KI and their mixture with $AgNO_3$
2. Thermodynamics of a chemical reaction by EMF-method.
3. Determination of (a) Standard electrode potential & (b) Activity Coefficient.

F. Conductometry

1. Verification of Debye-Huckel-Onsagar law.
2. Precipitation titration of $BaCl_2$ and K_2SO_4/ $(NH_4)_2SO_4$
3. Estimation of the concentrations of H_2SO_4, CH_3COOH and $CuSO_4$ in a mixture.

G. Dynamic Electrochemistry

1. To estimate the surface area of a working electrode through chronoamperometry and chronocoulometry.
2. Using Cyclic Voltammetry to determine the formal potential and diffusion coefficient of $[Fe(CN)_6]^{3-}$.
3. Use cyclic voltammetry to determine the concentration of acetaminophen in a given sample.

H. Kinetics

1. Kinetic Investigation of BZ-Oscillatory reaction.
2. Kinetic study of enzyme catalyzed reaction (effect of pH and Temperature).

I. Viscometry and densitometery

1. Determination of Mol. Mass of a Polymer (Polyv inyl alcohol) using viscosity method.
2. To explore the nature of chemical bonding (head-head and Head tail linkage of monomers) in polyvinyl alcohol using Viscometry.
3. Determination of partial molar volume of sodium chloride solutions as a function of concentration from density measurements.

Books Recommended

1. Practical Physical Chemistry --- Findley revised by Kitchner.(Longman, 1971)
2. Experimental Physical Chemistry, A. M. Halpern, G. C. McBane, (Freeman, 2006)
3. Experiments in Physical Chemistry, 5th ed. --- Schoemaker et al. (MGH, 2003)
4. Experimental Electrochemistry---R. Holze (Wiley-VCH, 2009).

Course No: CH17413DCE

Title: Supramolecular Chemistry (02 Credits)

***Max. Marks:** 50* | ***Duration:** 32 Contact hours*

***Ist Unit Exam:** 25 marks* | ***IInd Unit (Term end) Exam:** 25 marks*

Unit-I Supramolecular Interactions (08 Contact hours)

Definition and Development of Supramoleclar Chemistry. Nature of Supramolecular Interactions.

Hard Soft Acid Base Concept- Concept, Classification, Symbiosis. Utility in drug design and molecular recognition. Soft Ligands for Soft Metal Ions-Mixed Crown Ethers and Mixed Cryptands.

Unit-II Supramolecular Receptors (08 Contact hours)

Cation Receptors: Supramolecular Cation Coordination Chemistry, EDTA- The Supramolecular Host. Introductory account of Cation Receptors - Podands, Corands, Cryptands, Spherands and Calixarenes.

Anion Receptors: Scope and Challenges, Anion Hydrophobicity-Hofmeister Series, Introductory Account of Anion Receptors - Cyclophanes, Pyrolles, Azacrowns and Metal Based receptors. Hydride Sponge and Anticrowns.

Ion-Pair Receptors: Concept and Significance

Unit-III Crystal engineering and Supramolecular Motiffs (08 Contact hours)

Crystal Engineering: Introduction, Tectons and Synthons. Hydrogen Bond- Introduction, Criteria

Nature and Importance.

Self Assembly: Scope and Objectives. Concepts and Classification. Introductory Account of Coordination Capsules, Catenenes, Rotaxenes and Molecular Knots.

Unit-IV Network Solids and Molecular Devices (08 Contact hours)

Network Solids: Concepts and Classification, Network Topology. Zeolites: Structure, utility and limitations. Metal Organic Frameworks-Introduction and application in catalysis and Gas storage.

***Molecular Devices*:** Philosophy of Molecular Devices, Photophysical Fundamentals and Mechanism of Energy and Electron Transfer, Introductory Account of Molecular Wires, Molecular Switches and Molecular Motors.

Books 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, Ist 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. Chemical Reviews. Vol. 115, Issue 15, year **2015**, Pages 6999-8156
8. Introduction: Supramolecular Chemistry. F. Huang and E. V. Anslyn. Chem. Rev. **2015**, 115, 6999−7000.
9. Supramolecular materials. D. B. Amabilino, D. K. Smith and J. W. Steed. Chem. Soc. Rev., **2017**, 46, 2404—2420
10. A Bond by Other Name. G. R. Desiraju. Angew. Chem. Int. Ed. **2011**, 50, 52-59.
11. The Weak Hydrogen Bond: In Structural Chemistry and Biology. G. Desiraju, T. Steiner. **Oxford, IUCr Monograph on Crystallography**.

Course No: CH17414DCE
Title: Designing Organic Synthesis (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I (A) Oxidative and Reductive Processes in Organic Synthesis (8 Contact hours)

Oxidation**:** Introduction, Aromatisation of cycloalkanes and alkenes using metal catalysts and DDQ. Oxidation of Alcohols using chromic acid, DCC and Swern reagent. Oppenaur oxidation. Oxidation of ketones. Oxidation at activated carbon-hydrogen bond. Oxidation with Selenium dioxide. Prevost hydroxylation and its modification by Woodward.

Reduction**:** lntroduction. Reduction of Alkenes, Alkynes and Aromatic rings.

Reduction of carbonyl compounds: Clemmensen and Wolf-Kishner reductions. Reductions using $LiAlH_4$ and $NaBH_4$ Bouveault-Blanc reduction. Reduction of Epoxides, Nitro, Nitroso, Azo and Oxime groups. Reductions using Tributyl Tin Hydride.

(B) Protection and Interconversion of Functional Groups (8 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-II 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, α, β-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; Verlage VCH;1986.
3. Principles of Organic Synthesis 2nd edn;. R. O. C. Norman; Chapman and Hall; 1978.
4. Advanced Organic Chemistry Part B, 5th edn.; F. A. Carey and R.J Sundberg ; Springer; 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, 6lh Ed., J. March,; Wiley; 2012.
9. Organic Synthesis- The disconnection Approach; Sturat Warren; Wiley; 2013

Course No: CH17415DCE
Title: Computational Chemistry (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I

(a) Numerical solution of equations (8 Contact hours)

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

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

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

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

(b) Numerical differentiation and integration (8 Contact hours)

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

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

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

Unit-II

(a) Interpolation and Curve Fitting (8 Contact hours)

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

Lagrange's interpolation method, Newton's divided differences, Cubic spline, piece wise interpolation.

Least squares approximation, linear and quadratic.

(b) Use of Mathematica/Scilab for numerical solution of problems(8 Contact hours)

The mathematica package will be used for the solution of problems covered under the above three units.

Books Recommended

1. Data Reduction & Error Analysis, Bevington& Robinson, (McGraw-Hill, 2003)
2. Computational Chemistry, A. C. Norris, (Wiley.)
3. Computer Software Applications in Chemistry - P. C. Jurs, (John Wiley, 1996.)
4. Numerical Methods for Scientists and Engineers, H. M. Antie, (TMH,).
5. Numerical Recipes in Fortran/C, W.H. Press et al., (CUP,1992)
6. Applied Numerical Analysis, Gerald &Wheatly, (Pearson Education, 2002)
7. Mathematical Methods for Scientists and Engineers, D.A. McQuarie, Viva Books, 1st Ed., 2009.
8. Mathematica Manual.

Course No: CH17416DCE
Title: Seminar (02 Credits)

Presentation by a candidate on any topic chosen in consultation with the teacher incharge.

(25 Marks)

Manuscript (on the topic) submission (25 Marks)

Course No: CH17417GE
Title: Synthetic Polymers and their Applications (02 Credits)

Max. Marks: *50* — ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit (Term end) Exam:*** *25 marks*

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

Course No: CH17418GE
Title: Novel Materials (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

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

Block Copolymers: Introduction: classification, micellization of diblock 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, photoconductivity and sensors.

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

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

Luminesence and phosphors. Lasers - general principle of lasing action, Ruby laser, semiconducing 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 Nanofluids 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, Jeremy Ramsden and Ventus Publishing ApS, 2009.

Course No: CH17419OE
Title: Food Chemistry (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

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_2, 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; 3rd Ed.; Marcel Dekker, Inc. NY; 2005.
2. Food: The Chemistry of its components; T.P. Coultate; 3rd 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; 2nd ed.; Springer International Edition; 2005.

Course No: CH17413DCE

Title: Supramolecular Chemistry (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*

Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Supramolecular Interactions (08 Contact hours)

Definition and Development of Supramoleclar Chemistry. Nature of Supramolecular Interactions.

Hard Soft Acid Base Concept- Concept, Classification, Symbiosis. Utility in drug design and molecular recognition. Soft Ligands for Soft Metal Ions-Mixed Crown Ethers and Mixed Cryptands.

Unit-II Supramolecular Receptors (08 Contact hours)

Cation Receptors: Supramolecular Cation Coordination Chemistry, EDTA- The Supramolecular Host. Introductory account of Cation Receptors - Podands, Corands, Cryptands, Spherands and Calixarenes.

Anion Receptors: Scope and Challenges, Anion Hydrophobicity-Hofmeister Series, Introductory Account of Anion Receptors - Cyclophanes, Pyrolles, Azacrowns and Metal Based receptors. Hydride Sponge and Anticrowns.

Ion-Pair Receptors: Concept and Significance

Unit-III Crystal engineering and Supramolecular Motiffs (08 Contact hours)

Crystal Engineering: Introduction, Tectons and Synthons. Hydrogen Bond- Introduction, Criteria

Nature and Importance.

Self Assembly: Scope and Objectives. Concepts and Classification. Introductory Account of Coordination Capsules, Catenenes, Rotaxenes and Molecular Knots.

Unit-IV Network Solids and Molecular Devices (08 Contact hours)

Network Solids: Concepts and Classification, Network Topology. Zeolites: Structure, utility and limitations. Metal Organic Frameworks-Introduction and application in catalysis and Gas storage.

Molecular Devices**:** Philosophy of Molecular Devices, Photophysical Fundamentals and Mechanism of Energy and Electron Transfer, Introductory Account of Molecular Wires, Molecular Switches and Molecular Motors.

Books 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, Ist 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. Chemical Reviews. Vol. 115, Issue 15, year **2015**, Pages 6999-8156
8. Introduction: Supramolecular Chemistry. F. Huang and E. V. Anslyn. Chem. Rev. **2015**, 115, 6999−7000.
9. Supramolecular materials. D. B. Amabilino, D. K. Smith and J. W. Steed. Chem. Soc. Rev., **2017**, 46, 2404—2420
10. A Bond by Other Name. G. R. Desiraju. Angew. Chem. Int. Ed. **2011**, 50, 52-59.
11. The Weak Hydrogen Bond: In Structural Chemistry and Biology. G. Desiraju, T. Steiner. **Oxford, IUCr Monograph on Crystallography**.

Course No: CH17412DCE
Title: Advanced Laboratory Course in Physical Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *75 Marks.* ***Internal Assessment****: 25 Marks*

A. Tensiometry

1. Investigation of variation of surface tension of n-butanol and sodium chloride solutions with concentration and hence determination of their surface excess concentrations using Gibb's Adsorption Isotherm.
2. Determination of CMC value of a detergent using tensiometry.

B. Cryoscopy

1. Investigation of variation of freezing point depression with concentration & determination of molecular mass.
2. Determination of the degree of dissociation of a salt/weak acid in solution.
3. Determination of activity co-efficient from freezing point measurements.

C. Spectrophotometry

1. To study the complexation reaction between Fe(III) & salicylic acid.
2. Determination of pK value of an indicator.

D. Spectrofluorometry

1. To determine the rate constant for fluorescence quenching of anthracene or perylene by CCl_4 in ethanol.
2. Using pyrene as probe determine the cmc of a surfactant and site of solubilization of pyrene in the micelle through spectrofluorometry.

E. Potentiometry

1. Precipitation titration of KCl, KBr, KI and their mixture with $AgNO_3$
2. Thermodynamics of a chemical reaction by EMF-method.
3. Determination of (a) Standard electrode potential & (b) Activity Coefficient.

F. Conductometry

1. Verification of Debye-Huckel-Onsagar law.
2. Precipitation titration of $BaCl_2$ and K_2SO_4/ $(NH_4)_2SO_4$
3. Estimation of the concentrations of H_2SO_4, CH_3COOH and $CuSO_4$ in a mixture.

G. Dynamic Electrochemistry

1. To estimate the surface area of a working electrode through chronoamperometry and chronocoulometry.
2. Using Cyclic Voltammetry to determine the formal potential and diffusion coefficient of $[Fe(CN)_6]^{3-}$.
3. Use cyclic voltammetry to determine the concentration of acetaminophen in a given sample.

H. Kinetics

1. Kinetic Investigation of BZ-Oscillatory reaction.
2. Kinetic study of enzyme catalyzed reaction (effect of pH and Temperature).

I. Viscometry and densitometery

1. Determination of Mol. Mass of a Polymer (Polyv inyl alcohol) using viscosity method.
2. To explore the nature of chemical bonding (head-head and Head tail linkage of monomers) in polyvinyl alcohol using Viscometry.
3. Determination of partial molar volume of sodium chloride solutions as a function of concentration from density measurements.

Books Recommended

1. Practical Physical Chemistry --- Findley revised by Kitchner.(Longman, 1971)
2. Experimental Physical Chemistry, A. M. Halpern, G. C. McBane, (Freeman, 2006)
3. Experiments in Physical Chemistry, 5th ed. --- Schoemaker et al. (MGH, 2003)
4. Experimental Electrochemistry---R. Holze (Wiley-VCH, 2009).

Course No: CH17410DCE

Title: Advanced Laboratory Course in Inorganic Chemistry (04 Credits)

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

External Exam: *75 Marks.* | ***Internal Assessment****: 25 Marks*

A: - Inorganic Preparations: (5 Experiments)

- Preparation of tetraamminecarbonatocobalt (III) nitrate and its conversion to pentaamminecholorocobalt (III) chloride.
- Preparation of trans dicholoro bis (ethylenediamine) cobalt (III) chloride and its conversion to cis-isomer.
- Preparation of tris (ethylenediamine) nickel (II) chloride dihydrate and its conversion to bis (ethylenediamine) nickel (II) chloride.
- Preparation of bis (acetylacetonato) copper (II) dihydrate.
- Preparation of pentaamminecholorocobalt (III) chloride and study of Linkage isomers by its conversion to pentaamminenitritocobalt (III) chloride and to nitro isomer followed by IR Characterization.

B:- Total analysis of a Coordination compound for determination of various components present.

(1- Experiment)

C: - Separation by Column Chromatography and Estimations: (5 Experiments)

- Separation of Permanganate and Bichromate ions on Alumina column and their Estimation from Beer Law plots.
- Determination of lonisable chloride in a Complex by cation exchange column (separation followed by Mohr's titration of elute for estimation).
- Separation of Cobalt (II) and Nickel (II) on anion exchange column followed by estimation through EDTA titrations.
- Separation of two Cobalt (III) complexes viz $[Co(NH_3)_6]Cl_3$ and $[Co(NH_3)_5Cl]Cl_2$ on Silica column.
- Ion exchange separation of Hydration / ionization isomers of Chromium (III) Chloride ($CrCl_3$).

D: - Potentiometric Titrations: (6 Experiments)

- Standardization of an Iron (ii) solution with a standard dichromate solution over Pt & Calomel assembly.
- Determination of purity of Ce (IV) Sulphate with a standard Iron (II) solution over Pt & Calomel assembly.
- Estimation of Iodide with Standard $AgNO_3$ over Pt & Calomel assembly using I^- \ I2 redox couple.
- Simultaneous determinations of Chloride and Iodide ions with Standard $AgNO_3$ over Ag-Glass electrode assembly.
- Determination of the purity of $[Co(NH_3)_5Cl]Cl_2$ over Ag-Glass electrode assembly.
- Complexometric titration for determination of Ferro cyanide with standard Zinc (ii) solution and inorder to establish the composition of the complex $K_2Zn_3[Fe(CN)_6]_2$

E: - pH-metric Titrations: (2 Experiments)

- Quantitative analysis of Chromate Dichromate mixture by pH Titration.
- Purity of Acetyl Salicylic acid (Asprin) in a commercial tablet by pH Titration.

F: - Conductometric Titrations: (2 Experiments)

- To determine the solubility and solubility product of a sparingly soluble salt ($BaSO_4$) in water.
- To determine the basicity of sodium potassium tartarate by Conductometric method.

G:- Spectrophotometry: (5 Experiments)

- Determination of Iron (II) with 1,10-Phenanthroline.
- Determination of Phosphate by Molybdenum blue method.
- Determination of formula of Iron (III) thiocyanate complex by Job's Continuous variation method.
- Determination of composition of Iron (II)—2,2-bipyridyl complex by Mole ratio method.
- Determination of rate of Aquation of complex $[Co(NH_3)_5Cl]Cl_2$ in acidic medium.

H: - Flame Photometry: (2 Experiments)

- Simultaneous determination of Sodium and Potassium in the given mixture.
- Determination of Cadmium and Magnesium in tap water.

Books Recommended:

- Vogel's quantitative analysis 6 Edn. Mendham, Denny; Pearson Education 2002
- Synthesis and Technique in Inorganic chemistry , G. S.Girlomi; R.J. Angleci 3rd edn.; University Science Books.
- Synthesis and characterization of Inorganic compounds W.AJolly
- Inorganic syntheses Vols II, VI Academic Press.
- Experimental Inorganic / Physical Chemistry ; Mounir A. Malati Horwood/1999.
- Quantitative Chemical Analysis ; 5th edn.; Harris ; Freeman ; 1999.
- Advanced Practical Inorganic Chemistry ; Adams ; Raynor, Wiley ; 1995.
- Advanced Experimental Inorganic Chemistry ; Ayodha Singh ; Campus Books 2002.

Course No: CH17401CR
Title: Organo-Transition Metal Chemistry (04 Credits)

Max. Marks: *100* — ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Sigma Bonded Organometallic Compounds: (16 Contact hours)

Classification, Stability, Comparison to main Organometallic Compounds, Routes of synthesis, Reactions. Decomposition Pathways: Choice, α and β hydrogen transfer. Intramolecular elimination of alkane, Cyclometallation, Stability from bulky substituents, Agostic alkyls, Umpolung.Metal Hydride Complexes: Synthesis, Characterization and Chemical reactions, Non-classical Hydrides (Kubas complexes).

Unit-II Pi-bonded Organometallic Compounds: (16 Contact hours)

Classification, Structure and bonding in Metal- alkene, alkyne, allyl, 1,3-butadiene and Cyclobutadiene Complexes.

Sandwich Compounds: Characteristics; Classification, Synthesis, Reactions, 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.

Unit-III Catalytic Processes involving Transition Metal Organometallic Compounds: (16 Contact hours)

Mechanistic aspects: Oxidative addition, Insertion reactions Reductive elimination and water gas shift reaction (WGSR).

Catalytic mechanism of Hydrogenation, Hydroformylation, Oxidation and Isomerization of alkenes; Olefin metathesis.

Fischer-Tropsch Synthesis and Ziegler Natta polymerization of alkenes.

Asymmeteric and supported Organometallic Catalysis (brief idea)

Unit-IV Fluxional Organometallic Compounds and Synthetic Reactions involving Organo- metallics (16 Contact hours)

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 η^1 Cyclopentadienyls and η^3–allyls.

Stereochemical non rigidity in case of coordination numbers- 4 & 5 (cis-trans, atomic inversion, Berry Pseudorotation).

Synthetic Reactions involving Organo- metallics:

Reactions of coordinated ligands, carbon monoxide, alkyls, alkenes (Green, Mingo's rules).
Activation of small molecules: Carbon monoxide, Carbon dioxide and Alkanes.

Role of organo-iron as synthons, Carbon-Carbon coupling and its reactions (Suzuki and Heck).

Books Recommended:

1. The Organometallic Chemistry of Transition Metals; 2nd edn; Robert. H . Crabtree; Wiley; 1994.
2. Fundamental Transition Metal Organometallic Chemistry; Luke hart; Brooks / Cole; 1985.
3. Organometallic Chemistry; 2nd edn ; Mehrotra & Singh ; New age international 2000
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 press 1983.
9. Reaction Mechanism of Inorganic and Organometallic systems; 2nd edn.; Robert .b. Jordan 1998.
10. Inorganic Chemistry ; 4th edn.; Huheey ; E. Keiter & R. Keiter; Addison-Wesley ;1983
11. Modern Inorganic Chemistry; William. A. Jolly; McGraw Hill; 1985.

Course No: CH17402CR
Title: Photo-Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Basics of Photo-Chemistry (16 Contact hours)

Absorption; mechanism of absorption of light

Transition moment integral, Einstein's treatment, molar integrated absorption intensity, natural radiative lifetime & the calculation of life times.

Excitation; d-d transition, charge transfer & intraligand 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 diagramsdepicting excited states.

Frank Condon principle, shapes of absorption & emission bands.

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

Tools and Technique: Light source, measurement of light intensity, chemical actinometry. Flash photolysis.

Unit-II The Chemistry of Excited State Molecules (16 Contact hours)

Photochemical laws & quantum yield. Kinetics & quantum yield of photo-physical (radiative) and photo-chemical processes. Photochemical processes: primary, secondary, adiabatic & non- adiabatic. Properties of thexi states; Determination of dipole moments & acidity constants of excited state molecules.

Photosubstitution and photo reduction of Co (III) complexes.Photosubstitution reaction of Cr (III) and Rh (III) complexes.

Organometallic-Photochemistry: Reactions of metal carbonyls, cleavage of metal-metal bond.

Unit-III Redox Reactions by Excited Metal Complexes (16 Contact hours)

Energy transfer under conditions of weak and strong interaction. Excited state electron transfer. Marcus-Hush model.Conditions of the excited states to be useful as redox reactants. Photochemical electron transfer, [Ru (bipy)3]2+ and [Os (bipy)3]2+.

Photochemical supramolecular devices: devices for photo-induced energy or electron transfer, Devices for information processing, photo-chemically driven molecular machines.

Unit-IV Solar Energy-Prospects and Challenges (16 Contact hours)

Solar energy storage, solar energy conversion, Metal complex sensitizers and electron relays in photochemical splitting of water, Nitrogen fixation and CO_2 reduction. Inorganic photolithography.

Supramolecular photochemistry in natural systems: photosynthesis, bacterial photosynthesis and artificial photosynthesis.

Books Recommended:

1. Reaction Mechanisms of Inorganic and Organometallic Systems; 2nd edn.; Jordon; Oxford; 1998.
2. Mechanism of Inorganic Reactions; Katakis, Gordon; Wiley; 1987.
3. Inorganic Chemistry; 4* edn; Huheey; Harper & Row; 1990.
4. Mechanism of Inorganic Reactions, 2nd edn, Basalo, Pearson; Wiley Eastern, 1997.
5. Chemistry of Light; Suppan, Royal Society; 1994.
6. Photochemistry, Carol J. Wayne and Richard P. Wayne; Oxford University Press; 1996.
7. Fundamentals of Photochemistry; C Rohatgi, Mukhergi; Wiley Eastern.; 1992
8. Inorganic Photochemistry; J.Chem Edu.;Vol .60, No.10,1983.
9. Applications of Inorganic Photochemistry; J. Chem. Edu.; Vol.74, No 69. 1997.

Course No: CH17403CR
Title: Bio-Inorganic Chemistry (04 Credits)

Max. Marks: *100* | ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Iron Storage, Transport and Oxygen carriers: (16 Contact hours)

Structure and Coordinating sites in biologically important ligands: Proteins, Nucleotides and Lipids.

The transport mechanism: uniport, symport and antiport.

Ferritin and Transferrin: Structure, Metal binding sites; incorporation and release of iron.

Porphyrins: Introduction, characteristic absorption spectrum and salient characteristics.

Haemoglobin and Myoglobin: Structure, oxygen saturation curves; Mechanism of oxygen transport and storage.Bohr effect and cooperativity in haemoglobin.

Hemerythrin and Hemocyanin: Structure, Metal binding groups and Dioxygen binding. Synthetic oxygen carrier model compounds: Vaska's iridium complex: Cobalt complexes with micro and macrocyclic ligands and Schiff base ligands.

Unit-II Metallo-enzymes and Electron Carriers (16 Contact hours)

Enzyme, Apoenzyme, Coenzyme, Prosthetic group and Metalloenzymes, Mechanism of enzyme action.

Zinc enzymes:- Carboxypeptadiase and Carbonic Anhydrase : Introduction, Structure, Mechanism of action and their model compounds.

Biological chemistry of Molybednum: uptake of Molybednum; oxidation states and redox potentials in enzymes and oxygen atom transfer reactions.

Xanthine oxidase and Aldehyde oxidase: Structure and biological role.

Cobalt in Vitamin B_{12}: Introduction, Structure and Derivatives of B_{12} and mechanism of alkylation reaction. Role of vitamin B_{12}.

Electron Carriers: Rubredoxin & Ferridoxin (Structure and biological role).

Blue Copper proteins: Oxidases and Plastocyanin (Structure and biological role).

Unit-III Metal-ion Induced Toxicity and Chelation Therapy (16 Contact hours)

Toxic levels of different metals. Sources of metal ion poisoning (external sources and internal disorders).

Mechanism of metal ion induced toxicity:- Toxicity of Pb, Cd, Hg, As, and CN-Metal ion promoted Carcinogenesis and probable mechanism of action.

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 Metal Salts and Metal Complexes in Therapeutics (16 Contact hours)

Treatment of essential metal deficiencies: Iron, Copper and Cobalt.Metal salts as anti-acids, antiseptic and diuretics.

Gold compounds and Rhematoid arthiritis.

Anti-Cancer Drugs: cis-Platin and its derivatives. Structure-function relationship.

Complexes of Rhodium, Gold and Cobalt.

Anti-bacterial, Anti-viral and Anti-fungal activities of Metal Complexes: Labile and Robust metal complexes; Probable mechanism of action.

Books Recommended:

1. As listed for Course No. CHM—101 (Inorganic chemistry-M.Sc. 1st Semester! From serial No. 1 to 5.
2. Bio inorganic Chemistry -An introduction; Ochai, Allyn and Bacon; 1977.
3. Inorganic Bio-chemistry—Vol. 1&2; Eichhorn; Elsevier, 1973.
4. Inorganic Aspects of Biological and Organic Chemistry; Hanzilik; Academic; 1976.
5. The Inorganic Chemistry of Biological processes; 2nd edn.; Hughes ; Wiley; 1973.
6. A Text book of Medicinal aspects of Bio inorganic Chemistry; Das; CBS; 1990.
7. The Biological Chemistry of Elements; Frausto de Silva; Williams; Clarenden; 1991.
8. Principles of Bio inorganic Chemistry; Lippard, Berg; Univ. Science Books; 1994.
9. Inorganic Chemistry in Biology; Wilkins C & Wilkins G; Oxford; 1997.
10. Bio inorganic Chemistry ; K. Hussain Reddy; New Age International (P) Ltd; 2005.
11. Metal -Ions in Biochemistry; P. K. Bhattacharya; Narosa Publishing House; 2005.

Course No: CH17404CR
Title: Heterocyclic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Structure and Nomenclature of Heterocyclic compounds (16 Contact hours)

Introduction and significance of heterocycles in day to day life.

Nomenclature of Heterocycles: Monocyclic, bicyclic and polycyclic heterocycles, Hantzsch-Widman and replacement methods of nomenclature.

Structural features: Non-aromatic, aromatic and heteroaeromatic heterocycles.

Tautomerism in heterocycles, Meso-ionic systems.

Spectroscopic properties of heterocycles (UV,Visible and ^{1}HNMR).

Unit-II General Approach to Synthesis of Heterocyclic compounds (16 Contact hours)

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 quinoline, Bischler-Napieralki Isoquinoline,Knorr Pyrrole,Paal-Knorr , Fischer – Indole synthesis.

Unit-III Monocyclic Heterocycles (16 Contact hours)

Structure, Synthesis and Reactions of Oxirane, Thirane, Azetidine, Pyrrole, Furan, Thiophene, Diazenes, Pyrimidines,Pyridine.Chemistry of five membered heterocycles with two heteroatoms like 1,3-Azoles, 1,2- Azoles. Chemistry of Six membered rings like Azines and seven membered heterocycles like Azepine,Oxipene,Thiepins.

Unit-IV Bicyclic Heterocycles (16 Contact hours)

Structure, Synthesis and reactions of Benzo- fused heterocycles like Benzo-pyrrole, Benzo-furan,Benzo-thiophene, Quinoline, Isoquinoline, Chromones, Coumarins, Iso-Coumarins, 2 and 4-benzopyrones, Benzopyryllium salts and purines.

Books Recommended:

1. Heterocyclic Chemistry, 5th Ed. J.A.Joule and K.Mills, (Wiley-2010).
2. Essentials of Organic Chemistry, Paul M Dewick , (Wiley-2006).
3. Heterocyclic Chemistry, J.A. Joule and G.F.Smith , (Chapman and Hall-1996).
4. The Chemistry of Heterocycles Theophil Eicher and Siegfried Hauptmann , (George Thieme Verlag Stutt gart,New York -1995).
5. Heterocyclic Chemistry, Raj K. Bansal, (New Age International Publisher-2006).
6. Heterocyclic Chemistry, R.R.Gupta,M.Kumar,V.Gupta,(Springer-2006).

Course No: CH17405CR
Title: Chemistry of Natural Products (04 Credits)

***Max. Marks:** 100* — ***Duration:** 64 Contact hours*
***Ist Unit Exam:** 25 marks* — ***IInd Unit Exam:** 25 marks*
***End Term Exam (units III & IV):** 50 Marks*

Unit-I Terpenoids and Carotenoids (16 Contact hours)

Introduction, classification, general methods of isolation, separation.

Essential oils: Separation using Gas Liquid Chromatography and High Performance Liquid Chromatography. Physical, chemical and spectral methods of structure elucidation.

Structure determination, stereochemistry and synthesis of α-terpineol, abietic acid and β-carotene.

Unit-II Alkaloids (16 Contact hours)

Introduction, classification, nomenclature, qualitative tests, pharmaceutical applications and general methods of isolation. Physical, Chemical & Spectral methods of structure elucidation.

Stereochemistry, synthesis and biosynthesis of Quinine, Morphine and Reserpine.

Unit-III Steroids (16 Contact hours)

Introduction, nomenclature, classification & stereochemistry. Physical, Chemical & Spectral methods of characterization. Qualitative tests.

Cholesterol: Isolation, clinical significance, chemical properties, structure elucidation, total synthesis & relationship with bile acids.

Sex hormones: Introduction, isolation, clinical & commercial significance, color reactions, structure determination and partial synthesis of Oesterone, Androsterone, Testosterone and Progesterone.

Glucocorticoids & Mineral Corticoids: Introduction and partial synthesis of Cortisone, aldosterone and synthesis of cholecalciferol.

Unit-IV Natural Plant Pigments and Porphyrins (16 Contact hours)

Introduction, classification, physical, chemical, degradative and spectral methods of structure determination and biosynthesis (Acetate and Shikimic acid pathway)

Flavonoids: Isolation, separation and quantification. Antioxidant activity of flavonoids. Robinson's synthesis, Baker Venketraman synthesis, Kostanecki synthesis of flavanone and Flavanol.

Isolation, structure determination and synthesis of Cyanidin, Chrysin, Quercitin & Genestein.

Porphyrins: Structure determination and total synthesis of haemoglobin. Structural comparison with chlorophyll.

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. New Trends in Natural Product Chemistry, Atta-ur-Rahman (Harward Academic Press).
4. Chemistry of Natural Products, N.R. Krishnaswamy (University Press-1999).
5. Flavanoids; Oyvind M. Andersen and Kenneth R. Markhan. (Taylor & Francis -2006)

Course No: CH17406CR
Title: Bio-Organic and Medicinal Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

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

Vitamins:_ Source, structure and synthesis of vitamins – Vitamin A, Vitamin B-Complex (Thiamine riboflavin, folic acid); Vitamin B-12 (Structure only) Vitamin C, E, K, H and D.

Prostaglandins : Introduction and nomenclature, approaches to prostaglandin synthesis, cyclo-hexane, precursors-Woodward synthesis of PGF2a. Cyclo-heptane precursors - Corey's synthesis of prostoglandin's E & F.Their relationship with oxygenase I and II.

Nucleic Acids: Structure of nucleotide, nucleosides, RNA and DNA, role of nucleic acids in protein synthesis, genetic code and heredity. DNA finger printing

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

Enzymes : Introduction, nomenclature & classification.. Activation & inhibhion of enzymes. Mechanism of enzyme action- Fischer lock and key, koshlands induced fit hypothesis, displacement reactions & coupling of ATP. Enzyme mechanism of chymotrypsin lysozyme & carboxypeptidase.

Co-Enzymes: Cofactors derived from vitamins, coenzymes, prosthetic groups. Apoenzyme. Structure , biological function and mechanism of reactions catalsed by co-enzymes: coenzyme A, thiamine pyrophosphate. pyridoxal phosphate, NAD+, NADP+, FMN, FAD and Lipoic acid.

Unit-III **(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, carbonylic, thiols sulphides groups and introdction/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. Lipophillic constant, Hamett constant, steric parameters and Hansch analysis.

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

Antibiotics: Classifications-structural and mechanistic, cell wall biosynthesis inhibitors, protein synthesis inhibitors. Pencillins-classification and structures. Synthesis of Pencillins, V, G, chloroamphenicol.and ciprofloxacin. Tetracyclins.

Psychoactive Drugs: Introduction, CNS depressants, CNS stimulants, sedatives and hypnotics, barbutirates. Synthesis of diazepam, phenytoins and glutethisimide.

Anti-neoplastic drug: Introduction; cancer chemotherapy, carcenoolytic antibiotic, plant derived anti-cancer agents (Taxol)role of alkylative agents and antimetabolites in treatment of cancer, mitotic inhibitors (elementary idea).

Cardiovascular Drugs: Introduction, cardiovascular diseases, synthesis of Amylnitrate. sorbitrate, quinidine, verapanil, methyl dopa and atenolol

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, Biotechonolgy and Clinical Chemistry of Enzmyes. Trevor Palmer (EWP)
5. Organic Chemistry by I.L.Finar Vol. II (ELBS Longamnn)
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. Chemsitry of Natural Products. S.V. Bhat, B.A. Nagasampagi, M. Siva Kumar. Naroosa Publishing House, New Delhi.

Course No: CH17407CR
Title: Advanced Quantum Chemistry (04 Credits)

Max. Marks: *100* | ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Electronic Structure Theory, Hartree-Fock Method (16 Contact hours)

Review: Electronic Hamiltonian, antisymmetrized wave function, Slater determinant. Hartree-Fock self-consistent field method. One and two-electron integrals in the light of minimal basis H_2 system.

Hartree-Fock Equation, Fock, Coulomb and exchange operators and integrals, restricted Hartree-Fock formalism, Roothaan equation. The Fock matrix elements, Koopman's theorem, Slater-Condon rules. Matrix form of Roothaan equation, the SCF procedure.

Basis Sets: Slatter-type orbitals, Gaussian basis sets. Model SCF calculations on H_2 /HeH^{+}.

Unit-II Configuration Interaction and Semiempirical methods (16 Contact hours)

Configuration Interaction: Electron correlation, configuration state functions, configuration interaction (CI), Brillouin theorem, full and truncated CI theories- CID, CISD, CISDTQ methods; Size consistency problem. Moller-Plesset and Coupled Cluster methods.

Semiempirical methods: The ZDO approximation; the PPP method, brief idea of CNDO, INDO and NDDO methods. The MINDO, MNDO, AM1 and PM3 methods.

Unit-III Density Functional Methods and Molecular Properties (16 Contact hours)

Density Functional Theory:Electron probability density. Hohenberg-Kohn theorems, Kohn-Sham formulation of DFT, n- and v- representabilities, E_x&$E_c$functionals; the local density and local spin density approximations, gradient corrected and hybridfunctionals.
Brief idea of Molecular mechanics methods, force fields.

Molecular Properties*:* Potential energy surfaces; molecular geometry and its optimization, Hessian Matrix and normal modes, vibrational frequencies, thermodynamic properties. Dipole moments, atomic Charges.

Unit-IV Use of Quantum Chemistry Software: Gaussian (16 Contact hours)

A quick tour of GAUSSIAN Interface. Input to Gaussian. Model calculations illustrating various features of the package..

1. A single point energy calculation: HCHO /CH3.CHO,HCHOMOs.
2. Geometry Optimization: Input and Output for ethene, fluoroethene, propene conformers
3. Transition state optimization $CH_2O \rightarrow HCOH$
4. NMR properties of ethane, ethene and ethyne.
5. Frequency Calculations: Input, Formaldehyde frequencies, Normal modes, zero point energy, thermodynamic properties, polarizability, hyperpolarazability.
6. Stationary points characterization –C3H5F
7. Model Chemistries: Basis set effect on HF bond length

8. Selecting an appropriate theoretical method:
   a) Electron correlation and post SCF methods, limitations of Hartree-Fock theory: HF bond energy, Optimization of O_3.
   b) Density Functional Theory: CO_2 structure and atomization energy.
   c) Butane / Isobutane isomerization energy, rotational barrier in n-butane.

9. Chemical reactions and reactivity:
   a) Hydration enthalpy of the reaction $H^+ + H_2O \rightarrow H_3O^+$
   b) Potential energy surfaces. Reaction path following (IRC calculation)
   $CH_2O \rightarrow HCOH$
   c) Heat of formation of CO_2 via an isodesmic reaction
10. Solvation models: Formaldehyde Frequencies in Acetonitrile

Books Recommended

1. Quantum Chemistry, Ira. N. Levine, (Prentice Hall, 2009).
2. Quantum Chemistry, 2nd Edn , D. A. McQuarrie, (University Science Books, 2007).
3. Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedmann, (Oxford, 2008).
4. Quantum Chemistry and spectroscopy, Engel & Reid, Pearson (2007)
5. Modern Quantum Chemistry - Introduction to Advanced electronic structure theory - A. Szabo & N. S. Ostlund, (Macmillan, 1982, Dover 1996).
6. Molecular Modeling, Principles and Applications, A. R. Leach, Prentice-Hall, 2001
7. Modern Electronic Structure Theory, D. R. Yarkouy (ed). (World Scientific, 1995)
8. Ab Initio Molecular Orbital Theory, by Hehre, Radom, Schleyer and Pople, (Wiley)
9. Density Functional Theory of Atoms and Molecules, R.G. Parr and W. Yang, Oxford(1989).
10. GAUSSIAN Manual, Gaussian Inc
11. Exploring chemistry with electronic structure methods, Foresman J.B., Frisch A., Gaussian Inc

Course No: CH17408CR
Title: Advanced Electrochemistry and Statistical Mechanics (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Instrumental Methods in Electrochemistry (16 Contact hours)

Fundamentals: Electrode potential and its measurement, standard and formal electrode potentials, three electrode measurements, uncompensated resistance.

Overview of electrode Processes: Faradaic and Non-Faradaic processes, factors affecting electrode reaction rate. Mass transfer: Convection, migration, diffusion, Fick's 1st and 2^{nd} law of diffusion,

Electrochemical Techniques:

Electrophoresis: Factors affecting ion migration, electro-osmosis, theory and applications of capillary electrophoresis.

Potential Step Methods: Chronoamperometry, Chronocoulometry at macro electrodes; theory and applications. Cottrell equation. Controlled-Potential coulometry, Constant-Current coulometric titrations.

Potential Sweep Methods: Linear sweep Voltammetry and Cyclic Voltammetry at macro electrodes theory and applications, Diagnostic criteria of Cyclic Voltammetry.

Unit-II Applied Electrochemistry (16Contacthours)

Electrochemistry of redox enzymes: Direct and mediated electron transfer, Enzyme modified electrodes-challenges and applications. Mechanism and approach to bioelectrosynthesis, examples of bioelectro synthesis-oxidation of alcohols, synthesis of dihydroxy acetone phosphate, site specific oxidation of sugars, reduction of carbonyl compounds, hydrogenation.

Energy storage devices: Desirable characteristics of energy storage devices, Discharge plot, Ragone plot. Batteries: Measures of battery performance. Classical batteries (Lead Acid, Nickel-Cadmium, Zinc-Mangenese dioxide). Modern batteries (Zinc-Air, Nickel-Metal Hydride, Lithium Ion Batteries), Supercapacitors.

Fuel cells, types of fuel Cells, basic fuel cell operation, kinetics of fuel cell reactions. Alkaline, Phosphoric acid, Polymer Electrolyte membrane and direct MeOH fuel cell, biofuel cells.

Unit-III Classical Statistical Mechanics and Ensemble concept (16 Contact hours)

Equations of Motion; Newton, Lagrange and Hamiltonian. Classical partition function, phase space and the Liouville equation, Kinetic theory of gases, equi-partition of energy, Maxwell's velocity distribution.

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. Statistical Mechanical treatment of imperfect gases. Virial equation of state from grand

partition function, virial coefficients in the classical limit, second and third virial coefficients.

Unit-IV Applied Statistical Mechanics (16 Contact hours)

Quantum Statistics: Fermi-Dirac and Boson-Einstein statistics, Nuclear spin statistics, symmetry and nuclear spin, Ortho and Para nuclear spin states, Ortho and Para Hydrogen and Deuterium, CO.

Application of grand partition function to Boson-Einstein and Fermi-Dirac statistics. Ideal Fermi-Dirac gas: Electrons in metals, Ideal Photon gas: Black body radiation, influence of wavelength for the Planck distribution, Bose-Einstein condensation.

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. Electrochemical Methods Fundamentals and Applications, 2ndEdition, Allen J.Bard, Larry R. Faulkner, John Wiley and Sons, INC.
2. Physical Electrochemistry-Principles, Methods and Applications, Israel Rubinstein (Ed.) Marcel Dekker, Inc. New York.
3. Understanding Voltammetry, 2nd Edition, Imperial College Press.
4. Elements of Molecular and Biomolecular Electrochemistry, Jean-Michel Saveant, Wiley-Interscience.
5. Electrochemistry, 2nd Edition, Carl H. Hamann, Andrew Hammett, Wolf Vielstich,Wiley-VCH.
6. Modern Electrochemistry 2B, 2nd Edition, J. O`M. Bockris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.
7. Statistical Thermodynamics, M. C.Gupta ,(NewAgeInternational,1993).
8. Statistical Thermodynamics-Fundamentals and Applications, N.M. Laurendeau, Cambridge University Press, 2005.
9. Statistical Mechanics, D.A. McQuarrie, (Viva,2003).
10. Introduction to Statistical Thermodynamics, Chandler, (OUP, 1987).
11. Statistical Thermodynamics and Kinetic Theory, C. E. Hecht, (Dover,1990).
12. Statistical Mechanics –Principles and Applications, Hill, Dover, 1987.
13. Statistical Thermodynamics for Chemists, A. Ben-Naim, (Plenum, 1992).
14. An introduction to Statistical Thermodynamics, Hill, (Addison-wesley,1987).

Course No: CH17409CR
Title: Chemistry of Materials (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Surfactant mixtures, Stimuli responsive surfactants and block copolymers (16 Contact hours)

Surfactant-Surfactant Interactions: Mixed micelle formation, mixed monolayer formation, synergism, Clint and Rubingh's models of mixed micelle formation**.** Importance and practical applications of mixed surfactant systems.

Stimuli-Responsive Surfactants: Introduction and applications: Biosurfactants, redox, photochromic, thermoreversible, pH-sensitive, cleavable and magnetic surfactants.

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

Unit-II Hydrogels and microemulsions (16 Contact hours)

Hydrogels: Introduction, Types of Hydrogels, Preparation, Properties and characterization of Hydrogels, Biomedical applications of Hydrogels.

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

Unit-III Langmuir Blodgett Films, Liquid crystals and Fullerenes (16 Contact hours)

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.

Fullerenes: Fullerenes- History, bonding, properties, doped fullerenes, fullerenes as superconductors and fullerene related compounds (carbon nanotubes).

Unit-IV Optical materials and Ionic conductors (16 Contact hours)

Optical materials: Luminesence and phosphors. Lasers – general principle of lasing action, Ruby laser, Neodymium-YAG lasers, semiconducing lasers and quantum dot lasers. Nonlinear optical effects, second and third order harmonic generation, nonlinear optical materials.

Ionic Conductors: Introduction to ionic conduction and mechanism. Types of ionic conductors, mechanism of ionic conduction, interstitial jumps (Frenkel); vacancy

mechanism. Super-ionic conductors: Diffusion and transition superionic conductors and mechanism of conduction in superionic conductors; examples and applications of ionic conductors.

Books Recommended:

1. M. J. Rosen, J. T. Kunjappu, “Surfactants and Interfacial Phenomena”, John Wiley & Sons, New York, 4th Edition, 2012.
2. R. D. Vold and M. J. Vold, “Colloid and Interface Chemistry”, Addison-wesley, 1982.
3. .D. Y. Meyer, “Surfaces, Interfaces and Colloid”, VCH Publishers, Inc. 1991.
4. Jonsson, Lindmann, Homberg and Kronberg, “Surfactants and polymers in aqueous solution”, John Wiley and sons, 1998.
5. D. Fennell Evans, H. Wennerstrom, “The Colloidal Domain where physics, chemistry, biology and technology meet” VCH, New York, 1994.
6. Robert J. Hunter, “Foundations of Colloid Science”, Oxford University Press, New York, 2007.
7. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
8. I. W. Hamley, The Physics of Block Copolymers (Oxford University Press, Oxford, 1998.
9. N. Hadijichristidis, S. Pispas and G. A. Floudas Block Copolymers (Wiley, New York, 2003).
10. Introduction to Solids, Azaroff, Tata McGraw,1993.
11. SolidState Chemistry and its Applications, West, Wiley,1989.
12. The Physical Chemistry of Solids, Borg, Biens, Academic press, 1992.
13. Solid State Physics, N. W. Ashcroft and N. D. Mermin, Saunders college, 2001
14. Principles of Solid State, H. V. Keer, Wiley Eastern.
15. The Physics and Chemistry of materials, J.I. Gersten, F.W. Smith, John Wiley and sons, Inc. 2001.
16. Microemulsions: Background, New Concepts, Applications, Perspectives, C. Stubenrauch, Blackwell Publishing Ltd, 2009.
17. M. Sirousazar, M. Foroug, K. Farhad, Y. Shaabani and R. Molaei, Hydrogels: Properties, Preparation, Characterization and Biomedical, Applications in Tissue Engineering, Drug, Delivery and Wound Care, IN Advanced Healthcare Materials, Wiley online Library, 2014.

Course No: CH17410DCE
Title: Advanced Laboratory Course in Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *75 Marks.* ***Internal Assessment****: 25 Marks*

A: - Inorganic Preparations: (5 Experiments)

- Preparation of tetraamminecarbonatocobalt (III) nitrate and its conversion to pentaamminecholorocobalt (III) chloride.
- Preparation of trans dicholoro bis (ethylenediamine) cobalt (III) chloride and its conversion to cis-isomer.
- Preparation of tris (ethylenediamine) nickel (II) chloride dihydrate and its conversion to bis (ethylenediamine) nickel (II) chloride.
- Preparation of bis (acetylacetonato) copper (II) dihydrate.
- Preparation of pentaamminecholorocobalt (III) chloride and study of Linkage isomers by its conversion to pentaamminenitritocobalt (III) chloride and to nitro isomer followed by IR Characterization.

B:- Total analysis of a Coordination compound for determination of various components present.

(1- Experiment)

C: - Separation by Column Chromatography and Estimations: (5 Experiments)

- Separation of Permanganate and Bichromate ions on Alumina column and their Estimation from Beer Law plots.
- Determination of lonisable chloride in a Complex by cation exchange column (separation followed by Mohr's titration of elute for estimation).
- Separation of Cobalt (II) and Nickel (II) on anion exchange column followed by estimation through EDTA titrations.
- Separation of two Cobalt (III) complexes viz $[Co(NH_3)_6] Cl_3$ and $[Co (NH_3)_5 Cl] Cl_2$ on Silica column.
- Ion exchange separation of Hydration / ionization isomers of Chromium (III) Chloride ($CrCl_3$).

D: - Potentiometric Titrations: (6 Experiments)

- Standardization of an Iron (ii) solution with a standard dichromate solution over Pt & Calomel assembly.
- Determination of purity of Ce (IV) Sulphate with a standard Iron (II) solution over Pt & Calomel assembly.
- Estimation of Iodide with Standard $AgNO_3$ over Pt & Calomel assembly using I^- \ I2 redox couple.
- Simultaneous determinations of Chloride and Iodide ions with Standard $AgNO_3$ over Ag-Glass electrode assembly.
- Determination of the purity of $[Co (NH_3)_5Cl] Cl_2$ over Ag-Glass electrode assembly.
- Complexometric titration for determination of Ferro cyanide with standard Zinc (ii) solution and inorder to establish the composition of the complex $K_2Zn_3[Fe(CN)_6]_2$

E: - pH-metric Titrations: (2 Experiments)

- Quantitative analysis of Chromate Dichromate mixture by pH Titration.
- Purity of Acetyl Salicylic acid (Asprin) in a commercial tablet by pH Titration.

F: - Conductometric Titrations: (2 Experiments)

- To determine the solubility and solubility product of a sparingly soluble salt ($BaSO_4$) in water.
- To determine the basicity of sodium potassium tartarate by Conductometric method.

G:- Spectrophotometry: (5 Experiments)

- Determination of Iron (II) with 1,10-Phenanthroline.
- Determination of Phosphate by Molybdenum blue method.
- Determination of formula of Iron (III) thiocyanate complex by Job's Continuous variation method.
- Determination of composition of Iron (II)—2,2-bipyridyl complex by Mole ratio method.
- Determination of rate of Aquation of complex $[Co(NH_3)_5Cl]Cl_2$ in acidic medium.

H: - Flame Photometry: (2 Experiments)

- Simultaneous determination of Sodium and Potassium in the given mixture.
- Determination of Cadmium and Magnesium in tap water.

Books Recommended:

- Vogel's quantitative analysis 6 Edn. Mendham, Denny; Pearson Education 2002
- Synthesis and Technique in Inorganic chemistry , G. S.Girlomi; R.J. Angleci 3rd edn.; University Science Books.
- Synthesis and characterization of Inorganic compounds W.AJolly
- Inorganic syntheses Vols II, VI Academic Press.
- Experimental Inorganic / Physical Chemistry ; Mounir A. Malati Horwood/1999.
- Quantitative Chemical Analysis ; 5th edn.; Harris ; Freeman ; 1999.
- Advanced Practical Inorganic Chemistry ; Adams ; Raynor, Wiley ; 1995.
- Advanced Experimental Inorganic Chemistry ; Ayodha Singh ; Campus Books 2002.

Course No: CH17411DCE

Title: Advanced Laboratory Course in Organic Chemistry (04 Credits)

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

External Exam: *75 Marks.* — ***Internal Assessment****: 25 Marks*

1. **Multistep synthesis of drugs/ organic coinpouiuls involving name reactions**
   (1) Synthesis oflocal 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.
2. **Extraction/Estimation of Organic compounds from Natural sources**
   (1) Isolation of lycopene and β-carotene from tomato and their characterization using *uv*- spectroscopy.
   (2) Isolation of limonene from its natural source and physicochemical analysis.
   (3) Assay of Belladona for Hyoscyamine.
   (4) Assay of lemon from citric acid and vitamin-C
   (5) Isolation of cholesterol from gallstone
   (6) Assay of coke (soft drink)
3. **Column Chromatography**
   Separation of two component solid mixture. Identification of separated components using physical, chemical and spectral techniques.
4. **Spcctrophotomctric estimation** (UV/visible)
   (1) Vitamin-C (Ascorbic acid)
   (2) Caffeine from tea.
   (3) Cholesterol
   (4) Aspirin
5. **Elcctrophoresis/ Paper chromatography**
   Separation and identification of aminoacids by elcctrophoresis / Paper chromatography.
6. **Spcctroscopy**
   Identification of Organic compounds through interpretation of their spectra (UV, IR, PMR, CMR and Mass. Spectra to be provided).

Books Recommended :

1. Comprehensive Practical Organic Chemistry, V.K. Ahluwalia, Renu Aggarwal (Univ. Press India Limited -2000).
2. Vogel's Text Book of Practical Organic Chemistry, B.S.Furniss, A. J. Hannaford (AWL 5^{th} Ed.-1998).
3. Organic Laboratory Techniques , Donald .C. Pavia, Gary . M. Lampman (SCP 3rdEd.-1999)
4. Experiment Organic Chemistry, John.C. Gilbert., Stephen.F.Martin (SCP -1998)
5. Advanced Practical Organic Chemistry Vol. II, Jag Mohan (Himalaya Pub. House First Ed.-1992.

Course No: CH17412DCE
Title: Advanced Laboratory Course in Physical Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *75 Marks.* ***Internal Assessment****: 25 Marks*

A. Tensiometry

1. Investigation of variation of surface tension of n-butanol and sodium chloride solutions with concentration and hence determination of their surface excess concentrations using Gibb's Adsorption Isotherm.
2. Determination of CMC value of a detergent using tensiometry.

B. Cryoscopy

1. Investigation of variation of freezing point depression with concentration & determination of molecular mass.
2. Determination of the degree of dissociation of a salt/weak acid in solution.
3. Determination of activity co-efficient from freezing point measurements.

C. Spectrophotometry

1. To study the complexation reaction between Fe(III) & salicylic acid.
2. Determination of pK value of an indicator.

D. Spectrofluorometry

1. To determine the rate constant for fluorescence quenching of anthracene or perylene by CCl_4 in ethanol.
2. Using pyrene as probe determine the cmc of a surfactant and site of solubilization of pyrene in the micelle through spectrofluorometry.

E. Potentiometry

1. Precipitation titration of KCl, KBr, KI and their mixture with $AgNO_3$
2. Thermodynamics of a chemical reaction by EMF-method.
3. Determination of (a) Standard electrode potential & (b) Activity Coefficient.

F. Conductometry

1. Verification of Debye-Huckel-Onsagar law.
2. Precipitation titration of $BaCl_2$ and K_2SO_4/ $(NH_4)_2SO_4$
3. Estimation of the concentrations of H_2SO_4, CH_3COOH and $CuSO_4$ in a mixture.

G. Dynamic Electrochemistry

1. To estimate the surface area of a working electrode through chronoamperometry and chronocoulometry.
2. Using Cyclic Voltammetry to determine the formal potential and diffusion coefficient of $[Fe(CN)_6]^{3-}$.
3. Use cyclic voltammetry to determine the concentration of acetaminophen in a given sample.

H. Kinetics

1. Kinetic Investigation of BZ-Oscillatory reaction.
2. Kinetic study of enzyme catalyzed reaction (effect of pH and Temperature).

I. Viscometry and densitometery

1. Determination of Mol. Mass of a Polymer (Polyv inyl alcohol) using viscosity method.
2. To explore the nature of chemical bonding (head-head and Head tail linkage of monomers) in polyvinyl alcohol using Viscometry.
3. Determination of partial molar volume of sodium chloride solutions as a function of concentration from density measurements.

Books Recommended

1. Practical Physical Chemistry --- Findley revised by Kitchner.(Longman, 1971)
2. Experimental Physical Chemistry, A. M. Halpern, G. C. McBane, (Freeman, 2006)
3. Experiments in Physical Chemistry, 5th ed. --- Schoemaker et al. (MGH, 2003)
4. Experimental Electrochemistry---R. Holze (Wiley-VCH, 2009).

Course No: CH17413DCE

Title: Supramolecular Chemistry (02 Credits)

***Max. Marks:** 50* — ***Duration:** 32 Contact hours*

***Ist Unit Exam:** 25 marks* — ***IInd Unit (Term end) Exam:** 25 marks*

Unit-I Supramolecular Interactions (08 Contact hours)

Definition and Development of Supramoleclar Chemistry. Nature of Supramolecular Interactions.

Hard Soft Acid Base Concept- Concept, Classification, Symbiosis. Utility in drug design and molecular recognition. Soft Ligands for Soft Metal Ions-Mixed Crown Ethers and Mixed Cryptands.

Unit-II Supramolecular Receptors (08 Contact hours)

Cation Receptors: Supramolecular Cation Coordination Chemistry, EDTA- The Supramolecular Host. Introductory account of Cation Receptors - Podands, Corands, Cryptands, Spherands and Calixarenes.

Anion Receptors: Scope and Challenges, Anion Hydrophobicity-Hofmeister Series, Introductory Account of Anion Receptors - Cyclophanes, Pyrolles, Azacrowns and Metal Based receptors. Hydride Sponge and Anticrowns.

Ion-Pair Receptors: Concept and Significance

Unit-III Crystal engineering and Supramolecular Motiffs (08 Contact hours)

Crystal Engineering: Introduction, Tectons and Synthons. Hydrogen Bond- Introduction, Criteria

Nature and Importance.

Self Assembly: Scope and Objectives. Concepts and Classification. Introductory Account of Coordination Capsules, Catenenes, Rotaxenes and Molecular Knots.

Unit-IV Network Solids and Molecular Devices (08 Contact hours)

Network Solids: Concepts and Classification, Network Topology. Zeolites: Structure, utility and limitations. Metal Organic Frameworks-Introduction and application in catalysis and Gas storage.

***Molecular Devices*:** Philosophy of Molecular Devices, Photophysical Fundamentals and Mechanism of Energy and Electron Transfer, Introductory Account of Molecular Wires, Molecular Switches and Molecular Motors.

Books 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, Ist 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. Chemical Reviews. Vol. 115, Issue 15, year **2015**, Pages 6999-8156
8. Introduction: Supramolecular Chemistry. F. Huang and E. V. Anslyn. Chem. Rev. **2015**, 115, 6999−7000.
9. Supramolecular materials. D. B. Amabilino, D. K. Smith and J. W. Steed. Chem. Soc. Rev., **2017**, 46, 2404—2420
10. A Bond by Other Name. G. R. Desiraju. Angew. Chem. Int. Ed. **2011**, 50, 52-59.
11. The Weak Hydrogen Bond: In Structural Chemistry and Biology. G. Desiraju, T. Steiner. **Oxford, IUCr Monograph on Crystallography**.

Course No: CH17414DCE
Title: Designing Organic Synthesis (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I (A) Oxidative and Reductive Processes in Organic Synthesis (8 Contact hours)

Oxidation**:** Introduction, Aromatisation of cycloalkanes and alkenes using metal catalysts and DDQ. Oxidation of Alcohols using chromic acid, DCC and Swern reagent. Oppenaur oxidation. Oxidation of ketones. Oxidation at activated carbon-hydrogen bond. Oxidation with Selenium dioxide. Prevost hydroxylation and its modification by Woodward.

Reduction**:** lntroduction. Reduction of Alkenes, Alkynes and Aromatic rings.

Reduction of carbonyl compounds: Clemmensen and Wolf-Kishner reductions. Reductions using $LiAlH_4$ and $NaBH_4$ Bouveault-Blanc reduction. Reduction of Epoxides, Nitro, Nitroso, Azo and Oxime groups. Reductions using Tributyl Tin Hydride.

(B) Protection and Interconversion of Functional Groups (8 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-II 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, α, β-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; Verlage VCH;1986.
3. Principles of Organic Synthesis 2nd edn;. R. O. C. Norman; Chapman and Hall; 1978.
4. Advanced Organic Chemistry Part B, 5th edn.; F. A. Carey and R.J Sundberg ; Springer; 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, 6lh Ed., J. March,; Wiley; 2012.
9. Organic Synthesis- The disconnection Approach; Sturat Warren; Wiley; 2013

Course No: CH17415DCE
Title: Computational Chemistry (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I

(a) Numerical solution of equations (8 Contact hours)

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

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

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

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

(b) Numerical differentiation and integration (8 Contact hours)

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

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

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

Unit-II

(a) Interpolation and Curve Fitting (8 Contact hours)

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

Lagrange's interpolation method, Newton's divided differences, Cubic spline, piece wise interpolation.

Least squares approximation, linear and quadratic.

(b) Use of Mathematica/Scilab for numerical solution of problems(8 Contact hours)

The mathematica package will be used for the solution of problems covered under the above three units.

Books Recommended

1. Data Reduction & Error Analysis, Bevington& Robinson, (McGraw-Hill, 2003)
2. Computational Chemistry, A. C. Norris, (Wiley.)
3. Computer Software Applications in Chemistry - P. C. Jurs, (John Wiley, 1996.)
4. Numerical Methods for Scientists and Engineers, H. M. Antie, (TMH,).
5. Numerical Recipes in Fortran/C, W.H. Press et al., (CUP,1992)
6. Applied Numerical Analysis, Gerald &Wheatly, (Pearson Education, 2002)
7. Mathematical Methods for Scientists and Engineers, D.A. McQuarie, Viva Books, 1st Ed., 2009.
8. Mathematica Manual.

Course No: CH17416DCE
Title: Seminar (02 Credits)

Presentation by a candidate on any topic chosen in consultation with the teacher incharge.

(25 Marks)

Manuscript (on the topic) submission (25 Marks)

Course No: CH17417GE
Title: Synthetic Polymers and their Applications (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

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

Course No: CH17418GE
Title: Novel Materials (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

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

Block Copolymers: Introduction: classification, micellization of diblock 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, photoconductivity and sensors.

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

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

Luminesence and phosphors. Lasers - general principle of lasing action, Ruby laser, semiconducing 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 Nanofluids 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, Jeremy Ramsden and Ventus Publishing ApS, 2009.

Course No: CH17419OE
Title: Food Chemistry (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

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_2, 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; 3rd Ed.; Marcel Dekker, Inc. NY; 2005.
2. Food: The Chemistry of its components; T.P. Coultate; 3rd 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; 2nd ed.; Springer International Edition; 2005.

Course No. CH17104DCE
Title: Laboratory Course in Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *75 Marks.* ***Internal Assessment****: 25 Marks*

I. Preparation of Coordination compounds of Transition metals:

1. Theoretical appraise of first row Transition metal Coordination Chemistry.
2. Synthesis as a Laboratory Technique (Concepts, Calculations and Design of Synthetic procedures).
3. Selected preparations of the following coordination compounds with the specific objectives:

i) Mercurytetrathiocyanatocobaltate(II)	:	To visualize the complexation process.
ii) Tristhioureacopper(I)sulphate monohydrate	:	Insitu generation and Stabilization of unusual oxidation state and re-crystallization /crystal growing
iii) Hexaamminecobalt(III) chloride	:	Multistep synthetic procedure
iv) Trisethylenediaminecobalt(III) chloride	:	Two stage synthesis and aerial oxidation/Resolution of a racemic mixture
v) Ammonium dodeca molbedophosphate	:	Synthesis of a heteroploy metallate/ Bonding and structure.

II. 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.

III.

A. Qualitative Analysis by Semi micro Technique:

Discussion about the analysis scheme. Analytical groups and Group reagents. Scales of Analysis, Skill of semi micro technique. Chemistry involved in separation and identification of less familiar cations by semi micro analysis.

B. Identification of four less familiar cations from different analytical groups with simple and complex combinations:

(i) Group I and II A
(ii) Group I, II A and II B
(iii) Group IIA and II B
(iv) Group I and Group III
(v) Group II B and Group III
(vi) Group III only.

IV. Inorganic Quantitative Analyses:

A. **Gravimetry:**

i) Skill and importance of weighing in Chemistry, Gravimetreric 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.

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) Barium (Ba^{2+}) as BaSO4 and Zinc as $[ZnEDTA]^{2-}$ complex.

iii) Barium (Ba^{2+}) as $BaSO_4$ and Nickel (Ni^{2+}) as $[NiEDTA]^{2-}$ complex.

iv) Nickel (Ni^{2+}) as Ni $(dmg)_2$ complex and Magnesium (Mg^{2+}) as $[Mg\ EDTA]^{2-}$ complex.

v) Copper (Cu^{2+}) as CuSCN and Magnesium (Mg^{2+}) as $[MgEDTA]^{2-}$ complex.

Books Recommended:

1. Advanced Inorganic Chemistry, 5th ed. / 6th 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; 5th edn; Jeffery, Bassett; (ELBS, 1989).
4. Quantitative Analysis; 6th edn; Day, Underwood (Printice Hall, 1993).
5. Analytical Chemistry, 6th Ed; D. Christian, Wiley.
6. Quantitative Analysis; 6th edn; Day, Underwood (Printice Hall, 1993).

Course No: CH17101CR
Title: Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Stereochemistry and Bonding in the Compounds of Main Group Elements (16 Contact hours)

Valence bond theory: Energy changes taking place during the formation of diatomic molecules; factors affecting the combined wave function. Bent's rule and energetics of hybridization.

Resonance: Conditions, resonance energy and examples of some inorganic molecules/ions.

Odd Electron Bonds: Types, properties and molecular orbital treatment.

VSEPR: Recapitulation of assumptions, shapes of trigonal bypyramidal, octahedral and pentagonal bipyramidal molecules / ions. (PCl_5, VO_3^-, SF_6, $[SiF_6]^{2-}$, $[PbCl_6]^{2-}$ and IF_7). Limitations of VSEPR theory.

Molecular orbital theory: Salient features, variation of electron density with internuclear distance. Relative order of energy levels and molecular orbital diagrams of some heterodiatomic molecules /ions. Molecular orbital diagram of polyatomic molecules / ions.

Delocalized Molecular Orbitals: Butadiene, cyclopentadiene and benzene.

Detection of Hydrogen Bond: UV-VIS, IR and X-ray. Importance of hydrogen bonding.

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

Stepwise and overall formation constants. Inert & labile complexes. Stability of uncommon oxidation states.

Metal Chelates: Characteristics, Chelate effect and the factors affecting stability of metal chelates.

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-III Bonding 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 ML6; Effect of pi-bonding. Molecular orbital and energy level diagram for bonding in Ferrocene, Square-planar and Tetrahedral complexes.

Unit-IV Pi-acid Metal Complexes (16 Contact hours)

Transition Metal Carbonyls: Carbon monoxide as ligand, synthesis, reactions, structures and bonding of mono- and poly-nuclear carbonyls. Vibrational spectra of metal carbonyls for structural diagnosis.

Prepration, reactions, structure and bonding of transition metal nitrosyls, dinitrogen and dioxygen complexes.

Tertiary phosphine as ligand.

Books Recommended

1. Principles of Inorganic Chemistry; 1st edn.; Brain W. Pfennig; Wiley; 2015.
2. Advanced Inorganic Chemistry; 5th. and 6th edn; F.A. Cotton , G. Wilkinson; Wiley; 1998/1999.
3. Inorganic Chemistry; 4th edn; J. E. Huheey; E. A. Keiter; Harper Collins; 2009.
4. Inorganic Chemistry; G. Wulfsberg; Viva; 2002.
5. Chemistry of the Elements; 2nd edn; N. N. Greenwood, A. Earnshaw; Butterworth; 1997.
6. Inorganic Chemistry; 3rd edn; D. F. Shriver; P. W. Atkins; Oxford; 1999.
7. Inorganic Chemistry; K.F. Purcell, J.C Kotz; Saunders; 1977.
8. Coordination Chemistry; D. Banerjea; Tata McGraw Hill; 1993.

Course No: CH17102CR
Title: Organic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Delocalized Chemical bonding (16 Contact hours)

Overview: Inductive effect. Conjugation, Cross conjugation, Hyperconjugation–Isovalent and sacrificial hyperconjugations, Acids / Bases, Nucleophiles and Electrophiles. Resonance, Rules for writing resonance structures, Steric inhibition of resonance.

Tautomerism: Different types including valence 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.

Unit-II Reactive Intermediates and Determination of Reaction Mechanism (16 Contact hours)

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

Determination of Reaction Mechanism: Reaction Mechanism & Types of reactions. Determining reaction mechanism: Structure of Product, Transition states & Intermediates (Hammond postulate). Catalysis including acid and base catalysis, Specific acid and base catalysis. Fate of individual atoms (Isotope Labeling). Stereochemical course of reaction. Thermodynamic and kinetic evidences. Correlation of structure – reactivity.

Unit-III Stereochemistry: (16 Contact hours)

Chirality: Introduction, Chirality due to chiral centre. Molecules with more than one Chiral centres, Threo and erythro isomers. Convention for of assigning D, L & R, S configurations. Optical activity due to chiral axis, chiral plane and helicity. Chirality involving atoms other than carbon. Chirality in metallic complexes. Enantiotopic and diastereotopic atoms, groups and faces.

Asymmetric Synthesis: Introduction and principle of asymmetric synthesism. Principal categories of asymmetric synthesis. Use of chiral substrates. Diastero-selectivity in Aldol reactions. Sterospecificity and steroselectivity of enzymes.

Confirmations: Origin of conformational energy. Angle and Pitzer strain. Conformational analysis of cycloalkanes, and decalines. Effect of conformation on reactivity in acyclic and cyclic systems. Conformation of sugars & anomeric effect. Conformation of cyclohexene, cyclohexanones and bicycloheptane – a bridged system.

Unit-IV Aliphatic Nucleophilic Substitutions : (16 Contact hours)

Mechanism and stereochemical implications of S_N2, S_N1, S_Ni and Neighbouring Group Participation (by π and σ-bonds) reactions. Comparison of S_N1 and S_N2 reactions. Effect of substrate structure, attacking nucleophile, leaving group and solvent on the rates of S_N1 and S_N2 reactions. Mixed S_N1 and S_N2 reactions. Nucleophilic substitution at allylic, benzylic, aliphatic trigonal and vinylic carbons. Nucleophilic substitution in alcohols, Mitsunobu reactions. Nucleophilic substitutions on other elements. Functional group transformation using S_N2 reactions in organic synthesis. Nucleophilic substitutions in biological systems.

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

Aliphatic Electrophilic Substitutions: General mechanism of S_E1, S_E2 and S_Ei reactions. Mechanisms of reactions involving migration of double bond. Effect of substrate, leaving group and solvent on reactivity. Stork-Enamine reaction.

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 3rd Ed., S.M. Mukherjee and S.P. Singh. (Macmillan-1998).
4. Stereochemistry of Organic Compounds 2nd Ed., D. Nasipuri. (New Age Inter.- 2008)
5. Stereochemistry of Carbon Compounds - E.L.Eliel. (TMH -2007)
6. Stereochemistry of Organic Compounds 7th Ed. - P.S. Kalsi. (New Age Inter.- 2012).
7. Organic Chemistry - 2nd Ed., J. Hornback. (Brooks/Cole- 2006,
8. Organic Chemistry, 5th Ed., John McMurry. (Brooks/Cole-2000).
9. Advanced Organic Chemistry, 5th Ed., F.A Carey & R.J Sundberg (Springer-2007).
10. Organic Chemistry, 2nd Ed., Jonathan Clayden (OUP-2012)
11. Organic Chemistry, 11th Ed., Solomons, T.W.G., (Wiley-2015).

Course No: CH17103CR
Title: Physical Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

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)

Theories of Chemical Reactions: Activated complex theory of reaction rates, statistical & thermodynamic formulations, comparison with collision theory. Theories of unimolecular reactions (Lindman, Hinshelwood , RRK and RRKM theories), Introduction to potential energy surfaces.

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

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

Unit-IV Chemical kinetics-II (16 Contact hours)

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

Reactions in solutions: Diffusion controlled reactions (partial & full microscopic diffusion control), Ionic Reactions; Single & double sphere models of ionic reactions.

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

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

Books Recommended:

1. Physical Chemistry –P. W. Atkins, 9^{th} 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, 7^{th} Edition, Pearson, 2009.
5. Quantum Chemistry, R. K. Prasad, 2^{nd} Edition, New Age Publishers, 2001.
6. Physics and Chemistry of Interfaces, H-J, Butt, K. Graf and M. Kappl, 2^{nd} Edition, Wiley-VCH Verlag Gmbh and Co. KGaA, 2006.
7. Physical Chemistry of Surfaces, A. W. Adamson and A. P. Gast, 6^{th} Edition, John Wiley and Sons, Inc. 1997.
8. Chemical Kinetics, K. J. Laidler, 3^{rd} 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. CH17104DCE
Title: Laboratory Course in Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *75 Marks.* ***Internal Assessment****: 25 Marks*

I. Preparation of Coordination compounds of Transition metals:

1. Theoretical appraise of first row Transition metal Coordination Chemistry.
2. Synthesis as a Laboratory Technique (Concepts, Calculations and Design of Synthetic procedures).
3. Selected preparations of the following coordination compounds with the specific objectives:

i) Mercurytetrathiocyanatocobaltate(II)	:	To visualize the complexation process.
ii) Tristhioureacopper(I)sulphate monohydrate	:	Insitu generation and Stabilization of unusual oxidation state and re-crystallization /crystal growing
iii) Hexaamminecobalt(III) chloride	:	Multistep synthetic procedure
iv) Trisethylenediaminecobalt(III) chloride	:	Two stage synthesis and aerial oxidation/Resolution of a racemic mixture
v) Ammonium dodeca molbedophosphate	:	Synthesis of a heteroploy metallate/ Bonding and structure.

II. 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.

III.

A. Qualitative Analysis by Semi micro Technique:

Discussion about the analysis scheme. Analytical groups and Group reagents. Scales of Analysis, Skill of semi micro technique. Chemistry involved in separation and identification of less familiar cations by semi micro analysis.

B. Identification of four less familiar cations from different analytical groups with simple and complex combinations:

(i) Group I and II A
(ii) Group I, II A and II B
(iii) Group IIA and II B
(iv) Group I and Group III
(v) Group II B and Group III
(vi) Group III only.

IV. Inorganic Quantitative Analyses:

A. **Gravimetry:**

i) Skill and importance of weighing in Chemistry, Gravimetreric 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.

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) Barium (Ba^{2+}) as BaSO4 and Zinc as $[ZnEDTA]^{2-}$ complex.

iii) Barium (Ba^{2+}) as $BaSO_4$ and Nickel (Ni^{2+}) as $[NiEDTA]^{2-}$ complex.

iv) Nickel (Ni^{2+}) as Ni $(dmg)_2$ complex and Magnesium (Mg^{2+}) as $[Mg\ EDTA]^{2-}$ complex.

v) Copper (Cu^{2+}) as CuSCN and Magnesium (Mg^{2+}) as $[MgEDTA]^{2-}$ complex.

Books Recommended:

1. Advanced Inorganic Chemistry, 5th ed. / 6th 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; 5th edn; Jeffery, Bassett; (ELBS, 1989).
4. Quantitative Analysis; 6th edn; Day, Underwood (Printice Hall, 1993).
5. Analytical Chemistry, 6th Ed; D. Christian, Wiley.
6. Quantitative Analysis; 6th edn; Day, Underwood (Printice Hall, 1993).

Course No: CH17105DCE
Title: Symmetry and Group Theory (02 Credits)

***Max. Marks:** 50* — ***Duration:** 32 Contact hours*

***Ist Unit Exam:** 25 marks* — ***IInd Unit (Term end) Exam:** 25 marks*

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, Symmetry groups and group multiplication tables.

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 Orthoganality Theorm-elementary idea, consequences of the Great Orthogonolity Theorem. Reducible and Irreducible representations, Mullikan symbols for IRS. Character table-construction of character tables for C2v, C3v and C4v point groups.

Applications of group theory to IR and Raman spectroscopy, 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 and Polarity.

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.

Course No: CH17106DCE
Title: Infrared, Raman and Electronic Spectroscopy (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

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_2, O_2),

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. Physical Methods for Chemists; R.S.Drago; 2nd edn; Saunders; 1992.
2. Fundamentals of Molecular Spectrsocopy; C.N.Banwell, E.M.Mc Cash; 4th edn; Tata McGrawHill; 1994.
3. Physical chemistry; P. W. Atkins; 6th edition; Oxford University Press; 1998.
4. Electronic Absorption Spectroscopy and related techniques; D N Sathyanarayna; UniversitiesPress.
5. Introductory Raman Spectroscopy; J. R. Ferraro, K. Nakamoto & C. W Brown; 2nd edn; Academic Press 2005.
6. Theory and Applications of Ultraviolet Spectroscopy; H.H.Jaffe, M.Orchin; Wiley; 1962.
7. Molecular Spectroscopy; 1st edn; J L. McHale; Prentice Hall; 1999.
8. Modern Spectroscopy; J.M.Hollas; Wiley; 1987.
9. Basic Principles of Spectroscopy; R.Chang; McGraw Hill; 1971.
10. Structural Methods in Inorganic Chemistry; 2nd edn; E.A.V.Ebsworth, D.W.H.Rankin, S.Cradock; Blackwell; 1991.

Course No: CH17001GE
Title: Chemistry of the Environment (02 Credits)

Max. Marks: *50* — ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Soil and Hydrosphere (16 Contact hours)

Soil: Nature and Composition of soil – Air, Water, Inorganic components, organic matter and humus. Acid – Base and Ion exchange reactions in soil.

Wastes and pollutants in soil: Chemical degradation, photochemical reactions and biodegradation. Desertification, Deforestation and soil erosion.

Hydrosphere: Chemical Composition of Water Bodies: Lakes & rivers, Factors determining composition (thermal stratification, acid-base, pE concept).

Aquatic pollution: Inorganic, Organic, Pesticide, Agricultural, Industrial and Sewage.

Water quality parameters: Dissolved oxygen, Metals, Content of Chloride, Phosphate, Nitrate, and Microorganisms. Water quality standards.

Analytical Methods for determining BOD, DO, COD, and choice of methods for determining metals (As, Cd, Hg, Pb & Se).

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

Unit-II Atmosphere (16 Contact hours)

Chemical Composition of the Atmosphere: Particles, ions, radicals and their formation. Vertical profile of the atmosphere, Heat budget of earth's atmospheric system. Chemical and photochemical reactions in atmosphere, photochemical smog formation.

Oxides of N, C, S and their effects.

Ozone layer: Formation of ozone and mechanism of ozone depletion.

Pollution by chemicals: Chlorofluorocarbons, hydrocarbons and ozone.

Green house effect: Cause, source and impact on global climate.

Consequences of Green house effect and remedial measures.

Acid rain: Chemical aspects, adverse effects and control.

Books Recommended

1. Environmental Chemistry; 5th edn; Colin Baird; Freeman & Co; 2012.
2. Environmental Chemistry; 9th edn.S.E.Manahan; Lewis Publishers;2009
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 pollution; B.K.Sharma & H.Kaur; Goel Publishcrs;1996.
7. Environmental Chemistry; Nigel. J.Bunce; Wurez Publishers; 1991.
8. Environmental Toxicology; Ed.Rose; Gordon & Breach Science Publishers.

Course No: CH17002GE
Title: Surfactants and their Applications (02 Credits)

Max. Marks: *50* — ***Duration:*** *32 Contact hours*

Ist Unit Exam: *25 marks* — ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Self-Assembly of Surfactants (16 Contact hours)

***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 Systems (16 Contact hours)

a) **Mixed Surfactant systems**: Mixed micelle formation, mixed monolayer formation, synergism, various models of mixed micelle formation(Clint, Rubingh, Motamurra, Blankschtein, and Rubing-Holland models) 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. Characterization of polymer- surfactant systems by various techniques like viscosity, light scattering, spectroscopic and conductance measurements. 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. Physical Chemistry; P.W. Atkins; ELBS; Oxford; 1994.
3. Principles of Colloid and Surface Chemistry; P.C. Heimenz; Marcel Dekker Inc; New York; 1986.
4. Surfactants and Interfacial Phenomena; M. J. Rosen; John Wiley & Sons; New York; 1989.
5. Colloid and Interface Chemistry; R. D. Vold and M. J. Vold; Addison-Wesley; 1982.
6. Surfaces, Interfaces and Colloid; D. Y. Meyer; VCH Publishers; Inc; 1991.
7. Surfactants and polymers in aqueous solution; Jonsson, Lindmann, Homberg and Kronberg; John Wiley and sons; 1998.
8. Advances in Colloid and Polymer Science; B.K.Paul & S.P.Moulik, Current Science,Vol.80,p 990-,2001; Vol.78,p 99,1998.
9. Critical Reviews in Food Science and Nutrition; John Flanagan & Harjinder Singh, ,Vol. 46, pp221-237, 2006.
10. Advanced Drug Delivery Reviews; M. J. Lawrence & G.D.Rees; Vol, 45, p 898, 2000.
11. Energy Fuels; T. N. Dantas, A.A.D, Netoetal; DOI:10.1021/ ef900952y; 2010.

Course No: CH17001OE
Title: Chemistry in Everyday Life (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

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

(a) Water- An Amazing Chemical Stuff

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)

Course No: CH17106DCE
Title: Infrared, Raman and Electronic Spectroscopy (02 Credits)

Max. Marks: *50* — ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit (Term end) Exam:*** *25 marks*

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_2, O_2),

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. Physical Methods for Chemists; R.S.Drago; 2nd edn; Saunders; 1992.
2. Fundamentals of Molecular Spectrsocopy; C.N.Banwell, E.M.Mc Cash; 4th edn; Tata McGrawHill; 1994.
3. Physical chemistry; P. W. Atkins; 6th edition; Oxford University Press; 1998.
4. Electronic Absorption Spectroscopy and related techniques; D N Sathyanarayna; UniversitiesPress.
5. Introductory Raman Spectroscopy; J. R. Ferraro, K. Nakamoto & C. W Brown; 2nd edn; Academic Press 2005.
6. Theory and Applications of Ultraviolet Spectroscopy; H.H.Jaffe, M.Orchin; Wiley; 1962.
7. Molecular Spectroscopy; 1st edn; J L. McHale; Prentice Hall; 1999.
8. Modern Spectroscopy; J.M.Hollas; Wiley; 1987.
9. Basic Principles of Spectroscopy; R.Chang; McGraw Hill; 1971.
10. Structural Methods in Inorganic Chemistry; 2nd edn; E.A.V.Ebsworth, D.W.H.Rankin, S.Cradock; Blackwell; 1991.

Course No: CH17204DCE
Title: Laboratory Course in Organic Chemistry (04 Credits)

Max. Marks: *100* — ***Duration:*** *64 Contact hours*
External Exam: *80 Marks.* — ***Internal Assessment****: 20 Marks*

1. **Qualitative Analyses of Organic Compounds**
   (i) **Physical Properties:** Physical state, colour, odour, solubility behavior 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, Nitrocompounds and Hydrocarbons.
   (iii) **Preparation and recrystallization of the derivatives of above mentioned group of compounds.**
2. **Separation, Purification and identification of Organic compounds from a three component mixture:**
   (a) **Separation based on solubility in water and organic solvents.**
   (b) **Separation based on Chemical properties:** Solubility in Sodium bicarbonate, Sodium Hydroxide and Hydrochloric acid.
   (c) **Identification of individual components using physico-chemical properties**
3. **Detection of functional groups using IR spectroscopy (spectra to be provided)**
4. **Quantitative Estimation of the following compounds**
   (a) Glucose.
   (b) Glycine
   (c) Acetone
   (d) Phenol.
   (e) Ascorbic acid.

5. Organic Preparations

(a) Acetylation of Cholesterol or salicylic acid.

(b) Oxidation of Cyclohexanol by chromic acid to get adipic acid.

(c) Aldol condensation: Dibenzal acetone and benzaldehyde.

(d) Cannizarro's reaction of 4-Chlorobenzaldelyde.

(e) Aromatic electrophillic substitutions in benzene, benzoic acid or aniline.

(f) Beckman rearrangement starting from acetophenone.

(g) Haloform reaction: Preparation of Iodoform.

Books Recommended:

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

Course No: CH17201CR
Title: Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

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

Energy profile of a reaction; reactivity of metal complexes; inert and labile complexes.
Types of substitution reactions; mechanistic classification of substitution reactions:- Dissociative, Associative, Dissociative conjugate base and Interchange.
Empirical criteria to differentiate the mechanism of substitution reaction.
Substitution in octahedral complexes- Classification of metal ions based on water exchange rates. Metal-complex formation- the Eigen-Wilkins mechanism. Anation reactions.
Hydrolysis Reactions; Simple Acid hydrolysis, Acid catalysed and Base hydrolysis. Stereochemical changes in Octahedral Substitution Reactions.
Substitution reactions without breaking of metal-ligand bond.

Unit-III Mechanism of Ligand Substitution Reactions in Square-Planar complexes: (16 Contact hours)

Significance of the two-term rate^law, Mechanism, and Steric course of the substitution reactions.
Factors affecting the rate of substitution:- entering and leaving groups; nucleophilicity of entering group and the n_{pt} scale, central metal ion, solvent and the non-leaving groups.
The Trans effect;- Theories, applications in synthesis.
cis-trans isomerization in square planar complexes.

Unit-IV Organo Metallic Compounds (16 Contact hours)

Introduction, Nomenclature, classification and importance of organometallic compounds.
Nomenclature and Classification of Organometallic compounds.
Effective atomic number (18-Valance electron) rule and its significance.
Stability of Organometallic Compounds towards heat, oxidation and hydrolysis.
Preparation, Properties, Structure, bonding and applications of Alkyls and aryls of Li, B and Al.
Synthesis, Structure and bonding in Zeise's Salt.
Homogenous Catalysis using Organometallic Compounds: Catalysis, Terminology of Catalysis and Tolman Catalytic loop;
Oxidative addition, reductive elimination and migration (insertion) reactions.
Hydrogenation and Hydroformation reactions in alkenes.

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. CH17202CR
Title: Organic Chemistry (04 Credits)

Max. Marks: *100* | ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Aromatic Electrophilic Substitution (16 Contact hours)

Overview: Arenium ion mechanism, Sigma and pi – complexes, Energy profile diagram, Effect of leaving group. Orientation and reactivity in mono substituted benzene ring , *Ortho / Para ratio*, Ipso attack.

The Third substitution : Orientation of substitution in benzene ring with more than one substituent. Orientation in other ring systems. Carboxylation of aromatic rings with $COCl_2$ and amidation with NH_2COCl. Reversal of F.C. acylations. 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 mechanism (S_N1, S_NAr, Benzyne and $S_{RN}1$). Structure reactivity relationships. Effect of leaving group and attacking nucleophile. Mechanisms of Von-Richter, Sommelet-Hauser and Smiles rearrangements and Chichibabin reaction.

Free Radical Substitution:

Free radical substitution mechanisms. Mechanisms at an aromatic substrate. Neighbouring Group Assistance in free radical reactions, Reactivity for aliphatic and aromatic substrates. Reactivity in the attacking radical. Effect of solvent on reactivity.

Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sandmeyer reaction, free radical rearrangements and Hunsdiecker reaction.

Unit-II Addition to multiple bonds. (16 Contact hours)

Addition to carbon-oxygen double bonds:

Overview of reactivity carbonyl compounds: Mechanisms of addition of water , hydrogen cyanide, alcohols , amines , organometallic reagents and hydrides to aldehydes and ketones.

Mechanism of Wittig, Mannich , Aldol, Cross Aldol , Cannizarro's , Knoevenagel, Robinson annulation, Claisen, Dickman , Benzoin , Perkin and Stobbes reactions.

Addition to carbon-carbon multiple bonds:

General mechanism, reactivity, orientation and stereochemical implications of additions reactions involving electrophiles, nucleophiles and free radicals. Addition to cyclopropane ring. Hydrogenation of double/triple bonds and aromatic rings. Hydroboration, Ene-reaction, Michael reaction and Sharpless assymetric epoxidation.

Unit-III Molecular Rearrangements (16 Contact hours)

General mechanistic treatment of nucleophilic, electrophilic and free radical rearrangments. Nature of migration and migratory aptitude and memory effect. Detailed study of following rearrangements: Wagner-Meerwein, Pinacol- Pinacolone, Demyanov, Benzil-Benzilic acid, Favorskii, Arndt-Eistert, Neber, Hofmann, Curtius, Lossen, Schmidt, Beckmann, Baeyer-Villiger, Pyne and Dienone - phenol rearrangements.

Unit-IV Pericyclic reactions. (16 Contact hours)

Molecular orbital symmetry, Frontier orbitals of ethene, 1,3- butadiene, 1,3,5-hexatriene and allylic systems. HOMO, LUMO concept, FMO approach. Classification of Pericyclic reactions. Woodward Hofmann rules for the following pericyclic reactions. Cycloadditions: Thermal and Photochemical 2+2 and 4+2 cycloadditions. Suprafacial and antrafacial cycloadditions.

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

Sigmatropic rearrangements: Classification, [1,3], [1,5] and [3,3] sigmatropic shifts. Cope and Claisen rearrangements. Suprafacial and antrafacial shifts of hydrogen atom.

Books Recommended

1. Advanced Organic Chemistry Reactions, Mechanism and Structure, 4th Ed.,Jerry March. (Wiley, 1999).
2. Advanced Organic Chemistry 4th Ed. - F. A. Carey and R. J. Sundberg. (Plenum, 2001).
3. A Guide Book to Mechanism in Organic Chemistry 6th Ed.- Peter Sykes. (Longman, 1996).
4. Structure and Mechanism in Organic Chemistry 2nd Ed. - C. K. Ingold. (CBS, 1994).
5. Modern Organic Reactions 2nd Ed. - H.O. House (Benjamin, 1972)
6. Principles of Organic Synthesis 2nd Ed. - R.O.C. Norman (Chapmann Hall, 1978)
7. Reaction Mechanism in Organic Chemistry 3rd Ed. - S.M. Mykherjee and S.P. Singh. Macmillan, 1998).
8. Organic Chemistry - J. Hornback,pk. (Brooks/Cole, 1998).
9. Fundamentals of Organic Cbemjstry , 5th ed.- Solomons. (Wiley, 1992).
10. Organic Chemistry, 5th Ed.- John McMurry. (Brooks/Cole, 2000).

Course No: CH17203CR
Title: Physical Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I 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.

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.

Ion solvent Interactions*:* Non structural (Born) treatment and an introduction to structural (Ion-dipole, Ion-quadruple) 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.

Unit-III Biophysical Chemistry (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 (synthesis & hydrolysis), Principles of coupled reactions and their importance for living systems.

Biopolymers: Molecular forces and Chemical bonding in Bio-polymers, hydrophobic interactions, structure of proteins, protein folding and unfolding. Biological membranes, phase transitions in biological membranes. Donan effect and transport across biological membranes.

Binding of Ligands and metal Ions to bio-macromolecules, one binding site per macromolecule, n equivalent binding sites per macromolecule, binding of oxygen to myoglobin and hemoglobin.

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

Concept of distribution, thermodynamic probability and most probable distribution. Sterling approximation. Method of undetermined multipliers.

Distribution Laws: Derivation of Boltzmann distribution law, Bose-Einstein and Fermi-Dirac laws (without derivation) and their comparison with Boltzmann distribution law.

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

Books Recommended:

1. Physical Chemistry –P. W. Atkins, 9th Edition, 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, Lioyd L Lee, World Scientific, 2008.
7. An Introduction to Aqueous Electrolyte Solutions, Margaret Robson Wright, Wiley, 2007.
8. Modern Electrochemistry 1, 2A, 2nd Edition, J. O`M. Bokris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.
9. Physical Chemistry for the Biosciences, Raymond Chang, University Science Books, 2005.
10. Physical Chemistry for the Life Sciences,2nd Edition, Peter Atkins, Julio de Paula, Oxford University Press2015.
11. Statistical Thermodynamics, M.C.Gupta, New Age International, 1993.
12. Statistical Mechanics, Agarwal, Eisner, Wiley, 1991.

Course No: CH17204DCE
Title: Laboratory Course in Organic Chemistry (04 Credits)

Max. Marks: *100* — ***Duration:*** *64 Contact hours*
External Exam: *80 Marks.* — ***Internal Assessment****: 20 Marks*

1. **Qualitative Analyses of Organic Compounds**
   (i) **Physical Properties:** Physical state, colour, odour, solubility behavior 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, Nitrocompounds and Hydrocarbons.
   (iii) **Preparation and recrystallization of the derivatives of above mentioned group of compounds.**
2. **Separation, Purification and identification of Organic compounds from a three component mixture:**
   (a) **Separation based on solubility in water and organic solvents.**
   (b) **Separation based on Chemical properties:** Solubility in Sodium bicarbonate, Sodium Hydroxide and Hydrochloric acid.
   (c) **Identification of individual components using physico-chemical properties**
3. **Detection of functional groups using IR spectroscopy (spectra to be provided)**
4. **Quantitative Estimation of the following compounds**
   (a) Glucose.
   (b) Glycine
   (c) Acetone
   (d) Phenol.
   (e) Ascorbic acid.

5. Organic Preparations

(a) Acetylation of Cholesterol or salicylic acid.

(b) Oxidation of Cyclohexanol by chromic acid to get adipic acid.

(c) Aldol condensation: Dibenzal acetone and benzaldehyde.

(d) Cannizarro's reaction of 4-Chlorobenzaldelyde.

(e) Aromatic electrophillic substitutions in benzene, benzoic acid or aniline.

(f) Beckman rearrangement starting from acetophenone.

(g) Haloform reaction: Preparation of Iodoform.

Books Recommended:

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

Course No: CH17205DCE
Title: NMR and ESR Spectroscopy (02 Credits)

Max. Marks: *50* — ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I NMR Spectroscopy-I (08 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 (T1, T2). Shielding and deshielding of magnetic nuclei. Chemical shift, its measurement and factors influencing chemical shifts; local paramagnetic and diamagnetic shielding, neighboring group anisotropy and ring currents in aromatic systems

Unit-II NMR Spectroscopy-II (08 Contact hours)

Spin- Spin coupling, coupling constants. Examples.
Vicinal coupling and electron correlation. Chemical equivalence and magnetic equivalence.
Fermi contact and Dirac Vector Model. Effect of Chemical exchange on spectra.
Double resonance techniques; spin decoupling, nuclear overhauser enhancement.
Instrumentation; FT-NMR and its advantages. NMR studies of nuclei other than proton – ^{13}C, ^{19}F and ^{31}P.

Unit-III ESR spectroscopy-I (08 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

Unit-IV ESR spectroscopy-II (08 Contact hours)

Fermi contact, Spin polarization effects, Dipolar coupling, Mc Conell equation and calculation of spin densities in inorganic radicals such as $CO_2^{-\bullet}$, $CH_3^{\bullet}$, $BH_3^{-\bullet}$ and $F_2^{-\bullet}$.
Spin orbit coupling and significance of g tensors.
Zero field splitting and Kramer's degeneracy (fine structure),
Advance Applications

Books Recommended

1. Introduction to Spectroscopy; 3rd edn.; D. L. Pavia, G. M. Lampman, G. S. Kriz; Saunders-Thomson learning; 2001.
2. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry; R. V. Parish; Ellis Horwood; 1990.
3. Nuclear Magnetic Resonance; P. J. Hore; Oxford; 1995.
4. Principles of Instrumental Analysis; 4th edn.; D. A. Skoog, J. J. Leary; Saunders; 1992.
5. Physical Methods for Chemists; 2nd edn.; R. S. Drago; Saunders; 1992.
6. Basic Principles of Spectroscopy; R. Chang; McGraw Hill; 1971.
7. Introduction to Magnetic Resonance; A Carrington, A. D. McLachlan; Harper & Row; 1967.
8. NMR and Chemistry; 2nd edn.; J. W. Akitt; Chapman and Hall; 1983.

Course No: CH17206DCE
Title: Solid State Chemistry (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Structure and Theories of Solids (16 Contact hours)

Structure of solids: 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. *S*tructure 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, Colour centres, Dislocations and their types.

Theories of solids:

Free electron theory of metals**:** The Drude Model, Lorentz modification, Sommerfield Model; Fermi-Dirac distribution function, Density of states, electronic heat capacity, Hall effect.

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: CH17207GE
Title: Metal Ions in Living Systems (02 Credits)

Max. Marks: *50* — ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Alkali and Alkaline Earth Metal-ions in Biosystems (16 Contact hours)

Biomolecules and their Metal Coordination behavior.

Evidence of the presence of metal ions in biological systems (Direct / Indirect). Classification of metals and non-metals according to their action in biological systems.

Essential Elements: Concept of essentiality, criteria and classification of essential elements as per their role in living systems.

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.

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. Dioxygen transport (Haemocyanin).

Zinc in Biosystems: Lewis acid catalyst, Enzyme activator in vitamin B_{12}.

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

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

Antibacterial, Antiviral and Antifungal activities of metal complexes: Labile and Robust metal complexes; probable mechanism of action.

Books Recommended

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

Course No: CH17208GE
Title: Bio-Physical Chemistry (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Bioenergetics & Equilibrium in biological Systems (16 Contact hours)

Relevence of thermodynamics to Biological systems, Biochemists standard state, standard energy changes in biochemical reactions, ATP as energy currency of cell (synthesis & hydrolysis). Principles of coupled reactions and their importance for living systems.

Acid–base Equilibria: pH, pKa & pKb values. Dissociation of Amino-acids, isoelectric point. Buffer solutions, buffer capacity, effect of ionic strength & temperature, maintaining pH of blood.

Electrochemical equilibria: Standard redox potential, half- cell potentials of biological reactions, Nernst Equation.

Biological Membranes, Transport of ions across biological membranes, active and passive transport. Theory of membrane potential.

Unit-II Bio-electrochemistry, Kinetics & Spectroscopy (16 Contact hours)

Electrochemistry of Nerve conduction, medical applications of electrochemistry.

Renaturation of DNA as a second order reaction, Enzyme kinetics, Michaelis-Menton mechanism, competition & inhibition, multisubstrate systems, effect of substrate concentration, temperature and pH.

Fluorescence spectroscopy: Simple theory, excited state properties, florescence quenching, molecular rulers (FRET), single molecule florescence, applications in biological systems.

ORD and CD spectroscopy: Polarization of light and optical rotation, Optical rotatory dispersion and Circular dichroism, Circular dichroism of nucleic acids and proteins.

Books Recommended:

1. Physical Chemistry for life sciences; 2^{nd} edn.; P. W. Atkins and J.D. Paula; Oxford University Press; 2010.
2. Fundamentals of general Biological Chemistry; 4th edn.; John . R. Holum; Wiley; 1990.
3. Principles of biochemistry; 3rd edn.; David. L .Nelson, Michael .M.Cox; Worth Pub.; 2002.
4. Physical Chemistry, Principles and applications in biological systems. 4^{th}edn. Tinoco, Sauer, Wang, Puglisi. Pearson education, 2007.
5. Biophysical Chemistry; 2^{nd}edn.; Alan Cooper; RSC. Publishing; 2011.

Course No: CH17209OE
Title: Chemistry of Bio-molecules (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

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

Oils and Fats: Fatty acids and Triglycerides. Saturated and Unsaturated fatty acids (MUFA and PUFA). Rancidity of Oils & Fats. Absorption of toxic substances by fat.
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.
Minerals: Macro and Micro minerals. Their functions and diseases caused by their deficiencies.

Books Recommended

1. Organic Chemistry; 5th edn;. Vol.2,1.L. Finar (Addison Wesley Longman-2000).
2. Biochemistry, Biotechnology and Clinical Chemistry of Enzymes; Trevor Palmer (EWP). Organic Chemistry by I.L.Finar; Vol. II (ELBS Longamnn).
3. Lehninger's Principles of Bio-chemistry; D.L. Nelson; M.Cox Worth publications; 2000.
4. Introduction to Nucleic Acids and Related Natural Products; Ulbight; Oldborn Press.
5. Chemsitry of Natural Products; S.V. Bhat, B.A. Nagasampagi, M. Siva Kumar. Naroosa Publishing House; New Delhi.

Course No: CH17201CR
Title: Inorganic Chemistry (04 Credits)

Max. Marks: *100* | ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

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

Energy profile of a reaction; reactivity of metal complexes; inert and labile complexes.
Types of substitution reactions; mechanistic classification of substitution reactions:- Dissociative, Associative, Dissociative conjugate base and Interchange.
Empirical criteria to differentiate the mechanism of substitution reaction.
Substitution in octahedral complexes- Classification of metal ions based on water exchange rates. Metal-complex formation- the Eigen-Wilkins mechanism. Anation reactions.
Hydrolysis Reactions; Simple Acid hydrolysis, Acid catalysed and Base hydrolysis. Stereochemical changes in Octahedral Substitution Reactions.
Substitution reactions without breaking of metal-ligand bond.

Unit-III Mechanism of Ligand Substitution Reactions in Square-Planar complexes: (16 Contact hours)

Significance of the two-term rate^law, Mechanism, and Steric course of the substitution reactions.
Factors affecting the rate of substitution:- entering and leaving groups; nucleophilicity of entering group and the n_{pt} scale, central metal ion, solvent and the non-leaving groups.
The Trans effect;- Theories, applications in synthesis.
cis-trans isomerization in square planar complexes.

Unit-IV Organo Metallic Compounds (16 Contact hours)

Introduction, Nomenclature, classification and importance of organometallic compounds.

Nomenclature and Classification of Organometallic compounds.

Effective atomic number (18-Valance electron) rule and its significance.

Stability of Organometallic Compounds towards heat, oxidation and hydrolysis.

Preparation, Properties, Structure, bonding and applications of Alkyls and aryls of Li, B and Al.

Synthesis, Structure and bonding in Zeise's Salt.

Homogenous Catalysis using Organometallic Compounds: Catalysis, Terminology of Catalysis and Tolman Catalytic loop;

Oxidative addition, reductive elimination and migration (insertion) reactions.

Hydrogenation and Hydroformation reactions in alkenes.

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. CH17202CR
Title: Organic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Aromatic Electrophilic Substitution (16 Contact hours)

Overview: Arenium ion mechanism, Sigma and pi – complexes, Energy profile diagram, Effect of leaving group. Orientation and reactivity in mono substituted benzene ring , *Ortho / Para ratio*, Ipso attack.

The Third substitution : Orientation of substitution in benzene ring with more than one substituent. Orientation in other ring systems. Carboxylation of aromatic rings with $COCl_2$ and amidation with NH_2COCl. Reversal of F.C. acylations. 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 mechanism (S_N1, S_NAr, Benzyne and $S_{RN}1$). Structure reactivity relationships. Effect of leaving group and attacking nucleophile. Mechanisms of Von-Richter, Sommelet-Hauser and Smiles rearrangements and Chichibabin reaction.

Free Radical Substitution:

Free radical substitution mechanisms. Mechanisms at an aromatic substrate. Neighbouring Group Assistance in free radical reactions, Reactivity for aliphatic and aromatic substrates. Reactivity in the attacking radical. Effect of solvent on reactivity.

Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sandmeyer reaction, free radical rearrangements and Hunsdiecker reaction.

Unit-II Addition to multiple bonds. (16 Contact hours)

Addition to carbon-oxygen double bonds:

Overview of reactivity carbonyl compounds: Mechanisms of addition of water , hydrogen cyanide, alcohols , amines , organometallic reagents and hydrides to aldehydes and ketones.

Mechanism of Wittig, Mannich , Aldol, Cross Aldol , Cannizarro's , Knoevenagel, Robinson annulation, Claisen, Dickman , Benzoin , Perkin and Stobbes reactions.

Addition to carbon-carbon multiple bonds:

General mechanism, reactivity, orientation and stereochemical implications of additions reactions involving electrophiles, nucleophiles and free radicals. Addition to cyclopropane ring. Hydrogenation of double/triple bonds and aromatic rings. Hydroboration, Ene-reaction, Michael reaction and Sharpless assymetric epoxidation.

Unit-III Molecular Rearrangements **(16 Contact hours)**

General mechanistic treatment of nucleophilic, electrophilic and free radical rearrangments. Nature of migration and migratory aptitude and memory effect. Detailed study of following rearrangements: Wagner-Meerwein, Pinacol- Pinacolone, Demyanov, Benzil-Benzilic acid, Favorskii, Arndt-Eistert, Neber, Hofmann, Curtius, Lossen, Schmidt, Beckmann, Baeyer-Villiger, Pyne and Dienone - phenol rearrangements.

Unit-IV Pericyclic reactions. **(16 Contact hours)**

Molecular orbital symmetry, Frontier orbitals of ethene, 1,3- butadiene, 1,3,5-hexatriene and allylic systems. HOMO, LUMO concept, FMO approach. Classification of Pericyclic reactions. Woodward Hofmann rules for the following pericyclic reactions. Cycloadditions: Thermal and Photochemical 2+2 and 4+2 cycloadditions. Suprafacial and antrafacial cycloadditions.

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

Sigmatropic rearrangements: Classification, [1,3], [1,5] and [3,3] sigmatropic shifts. Cope and Claisen rearrangements. Suprafacial and antrafacial shifts of hydrogen atom.

Books Recommended

1. Advanced Organic Chemistry Reactions, Mechanism and Structure, 4th Ed.,Jerry March. (Wiley, 1999).
2. Advanced Organic Chemistry 4th Ed. - F. A. Carey and R. J. Sundberg. (Plenum, 2001).
3. A Guide Book to Mechanism in Organic Chemistry 6th Ed.- Peter Sykes. (Longman, 1996).
4. Structure and Mechanism in Organic Chemistry 2nd Ed. - C. K. Ingold. (CBS, 1994).
5. Modern Organic Reactions 2nd Ed. - H.O. House (Benjamin, 1972)
6. Principles of Organic Synthesis 2nd Ed. - R.O.C. Norman (Chapmann Hall, 1978)
7. Reaction Mechanism in Organic Chemistry 3rd Ed. - S.M. Mykherjee and S.P. Singh. Macmillan, 1998).
8. Organic Chemistry - J. Hornback,pk. (Brooks/Cole, 1998).
9. Fundamentals of Organic Cbemjstry , 5th ed.- Solomons. (Wiley, 1992).
10. Organic Chemistry, 5th Ed.- John McMurry. (Brooks/Cole, 2000).

Course No: CH17203CR
Title: Physical Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I 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.

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.

Ion solvent Interactions*:* Non structural (Born) treatment and an introduction to structural (Ion-dipole, Ion-quadruple) 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.

Unit-III Biophysical Chemistry (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 (synthesis & hydrolysis), Principles of coupled reactions and their importance for living systems.

Biopolymers: Molecular forces and Chemical bonding in Bio-polymers, hydrophobic interactions, structure of proteins, protein folding and unfolding. Biological membranes, phase transitions in biological membranes. Donan effect and transport across biological membranes.

Binding of Ligands and metal Ions to bio-macromolecules, one binding site per macromolecule, n equivalent binding sites per macromolecule, binding of oxygen to myoglobin and hemoglobin.

Unit-IV Statistical Thermodynamics (16 Contact hours)

Concept of distribution, thermodynamic probability and most probable distribution. Sterling approximation. Method of undetermined multipliers.

Distribution Laws: Derivation of Boltzmann distribution law, Bose-Einstein and Fermi-Dirac laws (without derivation) and their comparison with Boltzmann distribution law.

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

Books Recommended:

1. Physical Chemistry –P. W. Atkins, 9th Edition, 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, Lioyd L Lee, World Scientific, 2008.
7. An Introduction to Aqueous Electrolyte Solutions, Margaret Robson Wright, Wiley, 2007.
8. Modern Electrochemistry 1, 2A, 2nd Edition, J. O`M. Bokris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.
9. Physical Chemistry for the Biosciences, Raymond Chang, University Science Books, 2005.
10. Physical Chemistry for the Life Sciences,2nd Edition, Peter Atkins, Julio de Paula, Oxford University Press2015.
11. Statistical Thermodynamics, M.C.Gupta, New Age International, 1993.
12. Statistical Mechanics, Agarwal, Eisner, Wiley, 1991.

Course No: CH17204DCE
Title: Laboratory Course in Organic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *80 Marks.* ***Internal Assessment****: 20 Marks*

1. **Qualitative Analyses of Organic Compounds**
   (i) **Physical Properties:** Physical state, colour, odour, solubility behavior 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, Nitrocompounds and Hydrocarbons.
   (iii) **Preparation and recrystallization of the derivatives of above mentioned group of compounds.**
2. **Separation, Purification and identification of Organic compounds from a three component mixture:**
   (a) **Separation based on solubility in water and organic solvents.**
   (b) **Separation based on Chemical properties:** Solubility in Sodium bicarbonate, Sodium Hydroxide and Hydrochloric acid.
   (c) **Identification of individual components using physico-chemical properties**
3. **Detection of functional groups using IR spectroscopy (spectra to be provided)**
4. **Quantitative Estimation of the following compounds**
   (a) Glucose.
   (b) Glycine
   (c) Acetone
   (d) Phenol.
   (e) Ascorbic acid.

5. Organic Preparations

(a) Acetylation of Cholesterol or salicylic acid.

(b) Oxidation of Cyclohexanol by chromic acid to get adipic acid.

(c) Aldol condensation: Dibenzal acetone and benzaldehyde.

(d) Cannizarro's reaction of 4-Chlorobenzaldelyde.

(e) Aromatic electrophillic substitutions in benzene, benzoic acid or aniline.

(f) Beckman rearrangement starting from acetophenone.

(g) Haloform reaction: Preparation of Iodoform.

Books Recommended:

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

Course No: CH17205DCE
Title: NMR and ESR Spectroscopy (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I NMR Spectroscopy-I (08 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 (T1, T2). Shielding and deshielding of magnetic nuclei. Chemical shift, its measurement and factors influencing chemical shifts; local paramagnetic and diamagnetic shielding, neighboring group anisotropy and ring currents in aromatic systems

Unit-II NMR Spectroscopy-II (08 Contact hours)

Spin- Spin coupling, coupling constants. Examples.

Vicinal coupling and electron correlation. Chemical equivalence and magnetic equivalence.

Fermi contact and Dirac Vector Model. Effect of Chemical exchange on spectra.

Double resonance techniques; spin decoupling, nuclear overhauser enhancement.

Instrumentation; FT-NMR and its advantages. NMR studies of nuclei other than proton – ^{13}C, ^{19}F and ^{31}P.

Unit-III ESR spectroscopy-I (08 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

Unit-IV ESR spectroscopy-II (08 Contact hours)

Fermi contact, Spin polarization effects, Dipolar coupling, Mc Conell equation and calculation of spin densities in inorganic radicals such as $CO_2^{-\bullet}$, $CH_3^{\bullet}$, $BH_3^{-\bullet}$ and $F_2^{-\bullet}$.

Spin orbit coupling and significance of g tensors.

Zero field splitting and Kramer's degeneracy (fine structure),

Advance Applications

Books Recommended

1. Introduction to Spectroscopy; 3rd edn.; D. L. Pavia, G. M. Lampman, G. S. Kriz; Saunders-Thomson learning; 2001.
2. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry; R. V. Parish; Ellis Horwood; 1990.
3. Nuclear Magnetic Resonance; P. J. Hore; Oxford; 1995.
4. Principles of Instrumental Analysis; 4th edn.; D. A. Skoog, J. J. Leary; Saunders; 1992.
5. Physical Methods for Chemists; 2nd edn.; R. S. Drago; Saunders; 1992.
6. Basic Principles of Spectroscopy; R. Chang; McGraw Hill; 1971.
7. Introduction to Magnetic Resonance; A Carrington, A. D. McLachlan; Harper & Row; 1967.
8. NMR and Chemistry; 2nd edn.; J. W. Akitt; Chapman and Hall; 1983.

Course No: CH17206DCE
Title: Solid State Chemistry (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Structure and Theories of Solids (16 Contact hours)

Structure of solids: 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. *S*tructure 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, Colour centres, Dislocations and their types.

Theories of solids:

***Free electron theory of metals*:** The Drude Model, Lorentz modification, Sommerfield Model; Fermi-Dirac distribution function, Density of states, electronic heat capacity, Hall effect.

***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: CH17207GE
Title: Metal Ions in Living Systems (02 Credits)

Max. Marks: *50* — ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Alkali and Alkaline Earth Metal-ions in Biosystems (16 Contact hours)

Biomolecules and their Metal Coordination behavior.

Evidence of the presence of metal ions in biological systems (Direct / Indirect). Classification of metals and non-metals according to their action in biological systems.

Essential Elements: Concept of essentiality, criteria and classification of essential elements as per their role in living systems.

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.

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. Dioxygen transport (Haemocyanin).

Zinc in Biosystems: Lewis acid catalyst, Enzyme activator in vitamin B_{12}.

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

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

Antibacterial, Antiviral and Antifungal activities of metal complexes: Labile and Robust metal complexes; probable mechanism of action.

Books Recommended

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

Course No: CH17208GE
Title: Bio-Physical Chemistry (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Bioenergetics & Equilibrium in biological Systems (16 Contact hours)

Relevence of thermodynamics to Biological systems, Biochemists standard state, standard energy changes in biochemical reactions, ATP as energy currency of cell (synthesis & hydrolysis). Principles of coupled reactions and their importance for living systems.

Acid–base Equilibria: pH, pKa & pKb values. Dissociation of Amino-acids, isoelectric point. Buffer solutions, buffer capacity, effect of ionic strength & temperature, maintaining pH of blood.

Electrochemical equilibria: Standard redox potential, half- cell potentials of biological reactions, Nernst Equation.

Biological Membranes, Transport of ions across biological membranes, active and passive transport. Theory of membrane potential.

Unit-II Bio-electrochemistry, Kinetics & Spectroscopy (16 Contact hours)

Electrochemistry of Nerve conduction, medical applications of electrochemistry.

Renaturation of DNA as a second order reaction, Enzyme kinetics, Michaelis-Menton mechanism, competition & inhibition, multisubstrate systems, effect of substrate concentration, temperature and pH.

Fluorescence spectroscopy: Simple theory, excited state properties, florescence quenching, molecular rulers (FRET), single molecule florescence, applications in biological systems.

ORD and CD spectroscopy: Polarization of light and optical rotation, Optical rotatory dispersion and Circular dichroism, Circular dichroism of nucleic acids and proteins.

Books Recommended:

1. Physical Chemistry for life sciences; 2nd edn.; P. W. Atkins and J.D. Paula; Oxford University Press; 2010.
2. Fundamentals of general Biological Chemistry; 4th edn.; John . R. Holum; Wiley; 1990.
3. Principles of biochemistry; 3rd edn.; David. L .Nelson, Michael .M.Cox; Worth Pub.; 2002.
4. Physical Chemistry, Principles and applications in biological systems. 4thedn. Tinoco, Sauer, Wang, Puglisi. Pearson education, 2007.
5. Biophysical Chemistry; 2ndedn.; Alan Cooper; RSC. Publishing; 2011.

Course No: CH17209OE
Title: Chemistry of Bio-molecules (02 Credits)

Max. Marks: *50* — ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit (Term end) Exam:*** *25 marks*

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

Oils and Fats: Fatty acids and Triglycerides. Saturated and Unsaturated fatty acids (MUFA and PUFA). Rancidity of Oils & Fats. Absorption of toxic substances by fat.
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.
Minerals: Macro and Micro minerals. Their functions and diseases caused by their deficiencies.

Books Recommended

1. Organic Chemistry; 5th edn;. Vol.2,1.L. Finar (Addison Wesley Longman-2000).
2. Biochemistry, Biotechnology and Clinical Chemistry of Enzymes; Trevor Palmer (EWP). Organic Chemistry by I.L.Finar; Vol. II (ELBS Longamnn).
3. Lehninger's Principles of Bio-chemistry; D.L. Nelson; M.Cox Worth publications; 2000.
4. Introduction to Nucleic Acids and Related Natural Products; Ulbight; Oldborn Press.
5. Chemsitry of Natural Products; S.V. Bhat, B.A. Nagasampagi, M. Siva Kumar. Naroosa Publishing House; New Delhi.

Course No: CH17301CR
Title: Selected Topics in Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (Units III & IV): *50 Marks*

Unit-I Metal-ions in Biological Systems: (16 Contact hours)

The role of metal-ions in Metal-Protein systems; in trigger and control mechanisms; in structural context; as Lewis acid and as redox catalysts.

Biodistribution and biochemical role of essential trace and ultra-trace elements:- Fe, Zn, Cu, V, Cr, Mn, Ni, P, F and I. Effects of their deficiencies and treatment.

Antagonism and Synergism among essential trace elements.

Alkali and Alkaline earth metal ions (Na^+, K^+, Ca^{2+} & Mg^{2+}): Biological role; ligands and mechanism of ion transport (Facilitated transport, Carriers, Channeling and active transport of Cations).

Role of Lithium in mental health.

Chlorophyll: Structure and role of magnesium in photosynthesis.

Biological Nitrogen Fixation: Dinitrogen Complexes and their reactivity; Nitrogenase enzyme; Fixation via nitride formation.

Unit-II Bonding in Main Group Compounds (16 Contact hours)

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 Compounds (Borazine), Phosphorous–Nitrogen compounds (Cyclophosphazenes, polyphosphazenes and phosphonitrillic halides), Sulphur-Nitrogen compounds (polythiazyls and Sulphur Nitrides)

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 μ_s and μ_{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.

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.

Unit-IV NQR & Mossbauer Spectroscopy. (16 Contact hours)

Basic principles, Spectral parameters such as isomer shift, quadrupole splitting and magnetic splitting, spectrum display.

Application of the technique to the studies of (i) bonding and structure of Fe^{2+} and Fe^{3+} compounds including those of intermediate spin, (ii) Sn^{2+} and Sn^{4+} compounds— nature of M—L bond, coordination number and structure, (iii) detection of oxidation state and inequivalent MB atoms.

NQR isotopes, Nuclear quadruple moment; Electric field gradient; nuclear quadruple coupling constant; Effect of applied magnetic field, Applications.

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; IInd 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. Infrared and Raman Spectra: Inorganic and Coordination compounds ; K. Nakamoto; Wiley.
11. NMR, NQR and Mossbauer Spectrascopy in Inorganic Chemistry ; R.V.Parish; Ellis Horwood.

Course No: CH17302CR
Title: Organic Chemistry (Spectroscopy & Photochemistry) (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (Units III & IV): *50 Marks*

Unit-I Applications of Spectroscopy: (16 Contact hours)

Recapitulation of UV, IR Spectroscopy, Woodward-Fieser rule Characteristic absorptions of various functional groups. Interpretation of IR Spectra.

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. Mass Analyzer Determination of Molecular Formula, Role of Isotopes, Nitrogen Rule, Metastable Peak. Fragmentation pattern like Stevenson rule , initial ionization event, α-cleavage, inductive cleavage, two bond cleavage, Retro-Diels. Alder cleavage, McLaffertey Rearrangements. Fragmentation pattern of alkanes, alkenes, alcohols, phenols, aldehydes, ketones, Carboxylic acids, Amines, Problems based on Mass Spectroscopy. Some specific examples from natural products like flavanoids terpenes, steroids, alkaloids.

Unit-II Nuclear Magnetic Resonance 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 A_2, AB, AX, AB_2, AX_2, A_2B_2. Proton exchange, deuterium exchange, Peak broadening exchange

C-13 NMR : Carbon 13-chemical shifts , proton coupled and decoupled spectra. Nuclear overhouser, Effect, Off-Resonance De-coupling, A quick dip in to DEPT-45 , DEPT-90, DEPT-135.

Introduction to two-dimensional spectroscopy methods, Cosy techniques, HETCOR technique, OESY, combined structure problems.

Unit-III Photochemistry-I. (16 Contact hours)

Photochemical Reactions

Interaction of electromagnetic radiation with matter. Types of excitations. Singlet and triplet states and their lifetimes. Fate of excited molecule: Physical and chemical processes. Transfer of excitation energy: Sensitization and Quenching. Quantum yield. Types of photochemical reactions.

Photochemistry of alkenes

Geometrical isomerisations, cyclisation and dimerisation reactions. Photochemical reactions of 1,3- butadiene (excluding pericyclic reactions). Rearrangements of 1,4 and 1,5- dienes.

Photochemistry of saturated carbonyl compounds

Intramolecular reactions of saturated acyclic and cyclic carbonyl compounds. (Norrish type-I and Norrish type-II processess). Intermolecular cycloaddition reactions (Paterno- Buchi reaction).

Unit-IV Photochemistry –II. (16 Contact hours)

Photochemistry of unsaturated carbonyl compounds

Photochemical reactions of α, β-unsaturated carbonyl compounds. (H-Abstraction and isomerisation to β, γ-unsaturated carbonyl compounds). Photolysis of cyclic α, β-unsaturated ketones (dimerisation and lumiketone rearrangement) and cyclohexadienones.

Photochemistry of Aromatic compounds

Photoinduced isomerisations of benzene and its alkyl derivatives. 1,2 ; 1,3 and 1,4 photoaddition reactions of benzene. Nueleophilic photosubstitution reactions in aromatic compounds. Photo Fries-rearrangement of aryl esters and anilides.

Miscellaneous Photochemical reaction

Photolysis of organic nitrites and their synthetic utility (Barton reaction).

Photochemistry of vision.

Books recommened:

1. Spectrometric identification of Organic Compounds. 5th Ed., R.M.Silverstein, G.C.Bassler and T.C.Morill. (Jhon 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. Intoductory Photochemistry, A.Cox and T.Kemp (McGraw Hall-1971).
6. Organic Photochemistry, 2nd Ed., J.Coxon, and B.Halton (2nd Ed. Cambridge University press-1987).
7. Fundamentals of photochemistry, Rohtagi & Mukherjee (Wiley Eastern-1992).

Course No: CH17303CR
Title: Physical Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (Units III & IV): *50 Marks*

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 pi-bond-order. Alternant hydrocarbons, Naphthalene. 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-Fockself consistent field method. One and two-electron integrals in the light of minimal basis H_2 system

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 Electrochemistry-I (16 Contact hours)

Conductance of electrolyte solutions: Mobility of ions, mobility and conductivity, Einstein relations, dependence of molar conductance on concentration, estimation of K and Λ^0 for weak electrolytes, Theories of Conductance: Debye-Huckel-Onsager conductance equation and brief idea of its extension.

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, recent advances.

Semiconductor electrodes: Structure of seminconductor/electrolyte interface.

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

Theories of Heterogeneous Electron Transfer: Electron transfer at electrified interface at and away from equilibrium. Butller-Volmer equation, low and high field approximations, significance of transfer coefficient.

Electrochemistry in Materials Science: Corrosion, types and mechanism of corrosion, corrosion current, corrosion potential, Electrodics of corrosion in absence of Oxide films; Monitoring and inhibition of corrosion; cathodic and anodic protection, passivation.

Photoelectrochemistry: Band bending across Semiconductor/electrolyte solution interface, photoelectrochemistry across semiconductor/electrolyte interfaces, p-type photocathode, n-type-photoanode, surface effects in photoelectrochemitry, photoelectrochemical splitting of water, photoelectrochemical reduction of CO_2.

Books Recommended:

1. Physical Chemistry –P. W. Atkins, 9th Edition, 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, Tata McGraw 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. M. J. Rosen, J. T. Kunjappu, “Surfactants and Interfacial Phenomena”, John Wiley & Sons, New York, 4th Edition, 2012.
7. D. Y. Meyer, “Surfaces, Interfaces and Colloid”, VCH Publishers, Inc. 1991.
8. Jonsson, Lindmann, Homberg and Kronberg, “Surfactants and polymers in aqueous solution”, John Wiley and sons, 1998.
9. Molecular Thermodynamics of Electrolyte Solutions, Lioyd L Lee, World Scientific, 2008.
10. An Introduction to Aqueous Electrolyte Solutions, Margaret Robson Wright, Wiley, 2007.
11. Modern Electrochemistry 1, 2A,2B 2nd Edition, J. O`M. Bokris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.
12. Electrochemical methods, Fundamentals and Methods, A.J. Bard, L.R. Faulkner, Wiley, 1980.
13. Physical Electrochemistry- Fundamentals, Techniques and Applications, Eliezer Gileadi, Wiley-VCH 2011.
14. Electrochemistry, 2nd Edition, Carl H. Hamann, Andrew Hammett, Wolf Vielstich, Wiley-VCH.

Course No: CH17304DCE
Title: Laboratory Course in Physical Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *80 Marks.* ***Internal Assessment****: 20 Marks*

A. Conductometry

1. Determination of the composition of a mixture of HCl and CH_3COOH by titration with standard NaOH.
2. Determination of degree of dissociation of a weak acid.

B. Potentiometry

1. Determination of strength and pKa value of weak acid by titration with an alkali using quinhydrone electrode.
2. Titration of Fe (II) vs. $K_2Cr_2O_7$ and determination of standard redox potential of Fe^{2+}/Fe^{3+}.

C. pH-metry

1. Determination of pKa values of a tribasic acid by titration with an alkali.
2. Determination of degree of hydrolysis of aniline hydrochloride.

D. 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.

E. Spectrophotometry

1. Determination of composition of a binary mixture of $K_2Cr_2O_7$ and $KMnO_4$ or Cobalt (II) and Nickel (II) ions.
2. Spectrophotometric titration of Fe(II) vs. $KMNO_4$.

F. 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.

G. Viscometry

1. Investigation of variation of viscosity with conc. and determination of unknown concentration.
2. Determination of the radius of a molecule by viscosity measurement.

Books Recommended:

1. Practical Physical Chemistry, Findley, Kitchener, Longman, 1977.
2. Advanced Practical Physical Chemistry, Yadav , Goel Pub, 1994.
3. Experiments in Physical Chemistry, 5th ed., Schoemaker et al. , MGH, 1989.

Course No: CH17305DCE
Title: Chromatographic Techniques   (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

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; 5th Edition; F. W. Fifield, D. Kealey; Blackwell Sciences Ltd.; 2000.
2. Modern Analytical Chemistry; David Harvey; McGraw-Hill; 2000.
3. Chromatographic Methods; 5th edn. ; A. Braithwaite and F. J. Smith; Kluwer Academic Publishers.
4. Fundamentals of Analytical Chemistry; 6th 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: CH17306DCE
Title: Non-Equilibrium Thermodynamics (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

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 stationery 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 IrreversibleProcesses;DeGroot,Mazur;Dover;1986.
2. Introduction to Thermodynamics of Irreversible Processes; I.Prigogine; Wiley Interscience; 1967.
3. Thermodynamics for students of Chemsitry, Kuriacose, Rajaram, (S. ChandandCo., 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-equlibrium thermodynamics, 2^{nd} ed. Yasar Demirel. Elsevier, 2007.

Course No: CH17307GE
Title: Industrial Pollution and Green Chemistry (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Industrial Pollution and Environmental Toxicology (16 Contact hours)

Industrial Pollution: Cement, Sugar, Drug, Paper and pulp. Thermal power plants, Nuclear power plants and Polymers.

Radio nuclide analysis: Disposal of wastes and their management.

Principles of Toxicology, Dose Response Relationship, risk assessment and management.

Organochlorine Compounds: Accumulation and fate in biological systems. Toxicology of PCBs. Dioxins and Furans, Health effects in humans.

Environmental Estrogens.

Unit-II Green Chemistry (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 and Sonication.

Green Solvents and Reaction conditions: Supracritical fluids, aqueous reaction conditions, immobilized Solvents and irradiative reaction conditions.

Examples of Green materials, reagents and some specific reactions.

Books Recommended

1. Environmental Chemistry; 8^{th} edn.; S. E. Manahan; CRC Press; 2005.
2. Chemistry of the Environment; IInd edn.; T. G. Spiro and W. M. Stigliani; Prentice Hall; 2002.
3. Environmental Chemistry; IInd edn.; Colin Baird; Freeman & Co.; 1991.
4. Chemistry of the Environment; IInd Edn. R. A. Bailey; H. M. Clark; J. P. Ferris; S. Krause & R. L. Strong; Elsevier; 2005.
5. Environmental Chemistry; IInd edn.; Samir K. Banergi; Prentice- Hall; 2001.
6. Green Chemistry- Environment Friendly Alternatives; Rashmi Sangh & M. M Srivastava; Narosa; 2007.
7. Green Chemistry- An Introductory Text; IInd Edn.; Mike Lancaster; RSC; 2010.
8. Green Chemistry- Theory and Practice; P. T. Anastas and J. C. Warner; oxford; 2000.
9. Green Chemistry; Ist Edn.; Samuel Delvin; IVY Publishing House; 2008.
10. Green Chemistry- Environmentally Benign Reactions; V. K. Ahluwalia; Ane Books; 2006.

Course No: CH17308GE
Title: Bio-Organic Chemistry (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

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

(a) Chemical Origins of Biology

Bio organic chemistry: Introduction ,Basic consideration , Proximity effects in Organic Chemistry , Molecular rearrangments.

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 Nomeclature 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+ and NADP+), Flavin Nucleotides (FMN and FAD), Adenosine phosphate (ATP, ADP, AMP) .

Coenzyme A (CoA -SH) ,Thiamine Phosphate, Biotin, Tetrahydrofolate, Coenzyme B_{12} .

(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 Gregary Weiss; Taylor and francis. 2013.
2. Bio-organicchemistry : Harman Dugas 3rd ed.Springer (2010) .
3. Bio-organic chemistry J.Rohr ,Springer (2000).
4. Enzymes 2nd ed. T. Palmer and P. Bonner (2008).
5. Biochemistry :Donald Voet, Judith.G. Voet 2nd ed.Willey (1995)

Course No: CH17309OE
Title: Philosophy of Science (02 Credits)

Max. Marks: *50* — ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Representation (08 contact hours)

Laws of nature**:** Knowledge**, S**ources of knowledge, The rationalists, The empiricists, The Mathematical knowledge, Synthetic Knowledge, Science as knowledge source, Religion and science The Method of science, Induction versus deduction, Representation and reason, Probabilistic laws, Basic and derived laws,

Realism: Realism and its critics, Instrumentalism, Constructive empiricism, Laws and antirealism, Anti-realism and structure of science.

Unit-II Reason (08 contact hours)

Inductive Scepticism: Theory and observation, Dissolving the problem of Induction, Probability
and scientific inference, Kinds of Probability,

Inductive Knowledge: Reliabilist epistemology, reasoning with induction, Innate epistemic capacities and reasoning about induction, Internalism and justification.

Method and Progress: Methodology of scientific research programmes, Clinical trials and the scientific method, The content of discovery and the context of justification, Science without the scientific method, Method and the development of sciences, Paradigms and Progress.

Unit-III Classical Determinism and Probabilistic world (08 contact hours)

The Classical Mechanics: Mechanistic determinism, General principles; Action at a distance, Electric and magnetic forces, Failures of the classical mechanics;
Atomic structure, problem of radiation.

The birth of modern science**:** The photo-electric effect**,** The atomicity of radiation, Particle wave duality, waves of probability, Uncertainty principle, subject versus object, the fundamental laws of radioactivity, The new Quantum theory, wave mechanics, Diracs Quantum mechanics, The new philosophical principles, the probabilistic reasoning.

Unit-IV The Dawn of Modern Thinking (08 contact hours)

The arrow of Time: From Descarts to quantum theory, the relation of quantum theory to other natural sciences. Language and reality in modern science. The role of modern science in the present development of human thinking.

Books Recommended:

1. Philosophy of science; Alexander Bird; McGill-Queen's University Press.
2. Physics and Philosophy; W. Heisenberg; Harper Perennial Modern Classics.
3. Physics and Philosophy; Sir James Jeans; Cambridge University Press.
4. Reconstruction of religious thought in Islam; Muhammad Iqbal; Adam Publishers & Dodo Press.
5. Philosophy of natural science; Carl G. Hempel; Pearson.
6. The philosophy of science; David Papineaus; Oxford University Press.
7. Reality and Representation; David Papineaus; Blackwell Publication.
8. Belief, truth and knowledge; D.M. Armstrong; Cambridge University Press.
9. Modern epistemology; Nicholas Everitt and Alec Fisher; McGraw-Hill Higher Education.
10. The structure of scientific revolution; Thomas S. Kuhn; The University of Chicago Press

Course No: CH17401CR
Title: Organo-Transition Metal Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Sigma Bonded Organometallic Compounds: (16 Contact hours)

Classification, Stability, Comparison to main Organometallic Compounds, Routes of synthesis, Reactions. Decomposition Pathways: Choice, α and β hydrogen transfer. Intramolecular elimination of alkane, Cyclometallation, Stability from bulky substituents, Agostic alkyls, Umpolung.Metal Hydride Complexes: Synthesis, Characterization and Chemical reactions, Non-classical Hydrides (Kubas complexes).

Unit-II Pi-bonded Organometallic Compounds: (16 Contact hours)

Classification, Structure and bonding in Metal- alkene, alkyne, allyl, 1,3-butadiene and Cyclobutadiene Complexes.

Sandwich Compounds: Characteristics; Classification, Synthesis, Reactions, 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.

Unit-III Catalytic Processes involving Transition Metal Organometallic Compounds: (16 Contact hours)

Mechanistic aspects: Oxidative addition, Insertion reactions Reductive elimination and water gas shift reaction (WGSR).

Catalytic mechanism of Hydrogenation, Hydroformylation, Oxidation and Isomerization of alkenes; Olefin metathesis.

Fischer-Tropsch Synthesis and Ziegler Natta polymerization of alkenes.

Asymmeteric and supported Organometallic Catalysis (brief idea)

Unit-IV Fluxional Organometallic Compounds and Synthetic Reactions involving Organo- metallics (16 Contact hours)

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 η^1 Cyclopentadienyls and η^3–allyls.

Stereochemical non rigidity in case of coordination numbers- 4 & 5 (cis-trans, atomic inversion, Berry Pseudorotation).

Synthetic Reactions involving Organo- metallics:

Reactions of coordinated ligands, carbon monoxide, alkyls, alkenes (Green, Mingo's rules). Activation of small molecules: Carbon monoxide, Carbon dioxide and Alkanes.

Role of organo-iron as synthons, Carbon-Carbon coupling and its reactions (Suzuki and Heck).

Books Recommended:

1. The Organometallic Chemistry of Transition Metals; 2nd edn; Robert. H . Crabtree; Wiley; 1994.
2. Fundamental Transition Metal Organometallic Chemistry; Luke hart; Brooks / Cole; 1985.
3. Organometallic Chemistry; 2nd edn ; Mehrotra & Singh ; New age international 2000
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 press 1983.
9. Reaction Mechanism of Inorganic and Organometallic systems; 2nd edn.; Robert .b. Jordan 1998.
10. Inorganic Chemistry ; 4th edn.; Huheey ; E. Keiter & R. Keiter; Addison-Wesley ;1983
11. Modern Inorganic Chemistry; William. A. Jolly; McGraw Hill; 1985.

Course No: CH17402CR
Title: Photo-Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Basics of Photo-Chemistry (16 Contact hours)

Absorption; mechanism of absorption of light

Transition moment integral, Einstein's treatment, molar integrated absorption intensity, natural radiative lifetime & the calculation of life times.

Excitation; d-d transition, charge transfer & intraligand 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 diagramsdepicting excited states.

Frank Condon principle, shapes of absorption & emission bands.

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

Tools and Technique: Light source, measurement of light intensity, chemical actinometry. Flash photolysis.

Unit-II The Chemistry of Excited State Molecules (16 Contact hours)

Photochemical laws & quantum yield. Kinetics & quantum yield of photo-physical (radiative) and photo-chemical processes. Photochemical processes: primary, secondary, adiabatic & non- adiabatic. Properties of thexi states; Determination of dipole moments & acidity constants of excited state molecules.

Photosubstitution and photo reduction of Co (III) complexes.Photosubstitution reaction of Cr (III) and Rh (III) complexes.

Organometallic-Photochemistry: Reactions of metal carbonyls, cleavage of metal-metal bond.

Unit-III Redox Reactions by Excited Metal Complexes (16 Contact hours)

Energy transfer under conditions of weak and strong interaction. Excited state electron transfer. Marcus-Hush model.Conditions of the excited states to be useful as redox reactants. Photochemical electron transfer, [Ru (bipy)3]2+ and [Os (bipy)3]2+.

Photochemical supramolecular devices: devices for photo-induced energy or electron transfer, Devices for information processing, photo-chemically driven molecular machines.

Unit-IV Solar Energy-Prospects and Challenges (16 Contact hours)

Solar energy storage, solar energy conversion, Metal complex sensitizers and electron relays in photochemical splitting of water, Nitrogen fixation and CO_2 reduction. Inorganic photolithography.

Supramolecular photochemistry in natural systems: photosynthesis, bacterial photosynthesis and artificial photosynthesis.

Books Recommended:

1. Reaction Mechanisms of Inorganic and Organometallic Systems; 2nd edn.; Jordon; Oxford; 1998.
2. Mechanism of Inorganic Reactions; Katakis, Gordon; Wiley; 1987.
3. Inorganic Chemistry; 4* edn; Huheey; Harper & Row; 1990.
4. Mechanism of Inorganic Reactions, 2nd edn, Basalo, Pearson; Wiley Eastern, 1997.
5. Chemistry of Light; Suppan, Royal Society; 1994.
6. Photochemistry, Carol J. Wayne and Richard P. Wayne; Oxford University Press; 1996.
7. Fundamentals of Photochemistry; C Rohatgi, Mukhergi; Wiley Eastern.; 1992
8. Inorganic Photochemistry; J.Chem Edu.;Vol .60, No.10,1983.
9. Applications of Inorganic Photochemistry; J. Chem. Edu.; Vol.74, No 69. 1997.

Course No: CH17403CR
Title: Bio-Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Iron Storage, Transport and Oxygen carriers: (16 Contact hours)

Structure and Coordinating sites in biologically important ligands: Proteins, Nucleotides and Lipids.

The transport mechanism: uniport, symport and antiport.

Ferritin and Transferrin: Structure, Metal binding sites; incorporation and release of iron.

Porphyrins: Introduction, characteristic absorption spectrum and salient characteristics.

Haemoglobin and Myoglobin: Structure, oxygen saturation curves; Mechanism of oxygen transport and storage.Bohr effect and cooperativity in haemoglobin.

Hemerythrin and Hemocyanin: Structure, Metal binding groups and Dioxygen binding. Synthetic oxygen carrier model compounds: Vaska's iridium complex: Cobalt complexes with micro and macrocyclic ligands and Schiff base ligands.

Unit-II Metallo-enzymes and Electron Carriers (16 Contact hours)

Enzyme, Apoenzyme, Coenzyme, Prosthetic group and Metalloenzymes, Mechanism of enzyme action.

Zinc enzymes:- Carboxypeptadiase and Carbonic Anhydrase : Introduction, Structure, Mechanism of action and their model compounds.

Biological chemistry of Molybednum: uptake of Molybednum; oxidation states and redox potentials in enzymes and oxygen atom transfer reactions.

Xanthine oxidase and Aldehyde oxidase: Structure and biological role.

Cobalt in Vitamin B_{12}: Introduction, Structure and Derivatives of B_{12} and mechanism of alkylation reaction. Role of vitamin B_{12}.

Electron Carriers: Rubredoxin & Ferridoxin (Structure and biological role).

Blue Copper proteins: Oxidases and Plastocyanin (Structure and biological role).

Unit-III Metal-ion Induced Toxicity and Chelation Therapy (16 Contact hours)

Toxic levels of different metals. Sources of metal ion poisoning (external sources and internal disorders).

Mechanism of metal ion induced toxicity:- Toxicity of Pb, Cd, Hg, As, and CN-Metal ion promoted Carcinogenesis and probable mechanism of action.

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 Metal Salts and Metal Complexes in Therapeutics (16 Contact hours)

Treatment of essential metal deficiencies: Iron, Copper and Cobalt.Metal salts as anti-acids, antiseptic and diuretics.

Gold compounds and Rhematoid arthiritis.

Anti-Cancer Drugs: cis-Platin and its derivatives. Structure-function relationship.

Complexes of Rhodium, Gold and Cobalt.

Anti-bacterial, Anti-viral and Anti-fungal activities of Metal Complexes: Labile and Robust metal complexes; Probable mechanism of action.

Books Recommended:

1. As listed for Course No. CHM—101 (Inorganic chemistry-M.Sc. 1st Semester! From serial No. 1 to 5.
2. Bio inorganic Chemistry -An introduction; Ochai, Allyn and Bacon; 1977.
3. Inorganic Bio-chemistry—Vol. 1&2; Eichhorn; Elsevier, 1973.
4. Inorganic Aspects of Biological and Organic Chemistry; Hanzilik; Academic; 1976.
5. The Inorganic Chemistry of Biological processes; 2nd edn.; Hughes ; Wiley; 1973.
6. A Text book of Medicinal aspects of Bio inorganic Chemistry; Das; CBS; 1990.
7. The Biological Chemistry of Elements; Frausto de Silva; Williams; Clarenden; 1991.
8. Principles of Bio inorganic Chemistry; Lippard, Berg; Univ. Science Books; 1994.
9. Inorganic Chemistry in Biology; Wilkins C & Wilkins G; Oxford; 1997.
10. Bio inorganic Chemistry ; K. Hussain Reddy; New Age International (P) Ltd; 2005.
11. Metal -Ions in Biochemistry; P. K. Bhattacharya; Narosa Publishing House; 2005.

Course No: CH17404CR
Title: Heterocyclic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Structure and Nomenclature of Heterocyclic compounds (16 Contact hours)

Introduction and significance of heterocycles in day to day life.

Nomenclature of Heterocycles: Monocyclic, bicyclic and polycyclic heterocycles, Hantzsch-Widman and replacement methods of nomenclature.

Structural features: Non-aromatic, aromatic and heteroaeromatic heterocycles.

Tautomerism in heterocycles, Meso-ionic systems.

Spectroscopic properties of heterocycles (UV,Visible and ^{1}HNMR).

Unit-II General Approach to Synthesis of Heterocyclic compounds (16 Contact hours)

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 quinoline, Bischler-Napieralki Isoquinoline,Knorr Pyrrole,Paal-Knorr , Fischer – Indole synthesis.

Unit-III Monocyclic Heterocycles (16 Contact hours)

Structure, Synthesis and Reactions of Oxirane, Thirane, Azetidine, Pyrrole, Furan, Thiophene, Diazenes, Pyrimidines,Pyridine.Chemistry of five membered heterocycles with two heteroatoms like 1,3-Azoles, 1,2- Azoles. Chemistry of Six membered rings like Azines and seven membered heterocycles like Azepine,Oxipene,Thiepins.

Unit-IV Bicyclic Heterocycles (16 Contact hours)

Structure, Synthesis and reactions of Benzo- fused heterocycles like Benzo-pyrrole, Benzo-furan,Benzo-thiophene, Quinoline, Isoquinoline, Chromones, Coumarins, Iso-Coumarins, 2 and 4-benzopyrones, Benzopyryllium salts and purines.

Books Recommended:

1. Heterocyclic Chemistry, 5th Ed. J.A.Joule and K.Mills, (Wiley-2010).
2. Essentials of Organic Chemistry, Paul M Dewick , (Wiley-2006).
3. Heterocyclic Chemistry, J.A. Joule and G.F.Smith , (Chapman and Hall-1996).
4. The Chemistry of Heterocycles Theophil Eicher and Siegfried Hauptmann , (George Thieme Verlag Stutt gart,New York -1995).
5. Heterocyclic Chemistry, Raj K. Bansal, (New Age International Publisher-2006).
6. Heterocyclic Chemistry, R.R.Gupta,M.Kumar,V.Gupta,(Springer-2006).

Course No: CH17405CR
Title: Chemistry of Natural Products (04 Credits)

Max. Marks: *100* | ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Terpenoids and Carotenoids (16 Contact hours)

Introduction, classification, general methods of isolation, separation.

Essential oils: Separation using Gas Liquid Chromatography and High Performance Liquid Chromatography. Physical, chemical and spectral methods of structure elucidation.

Structure determination, stereochemistry and synthesis of α-terpineol, abietic acid and β-carotene.

Unit-II Alkaloids (16 Contact hours)

Introduction, classification, nomenclature, qualitative tests, pharmaceutical applications and general methods of isolation. Physical, Chemical & Spectral methods of structure elucidation.

Stereochemistry, synthesis and biosynthesis of Quinine, Morphine and Reserpine.

Unit-III Steroids (16 Contact hours)

Introduction, nomenclature, classification & stereochemistry. Physical, Chemical & Spectral methods of characterization. Qualitative tests.

Cholesterol: Isolation, clinical significance, chemical properties, structure elucidation, total synthesis & relationship with bile acids.

Sex hormones: Introduction, isolation, clinical & commercial significance, color reactions, structure determination and partial synthesis of Oesterone, Androsterone, Testosterone and Progesterone.

Glucocorticoids & Mineral Corticoids: Introduction and partial synthesis of Cortisone, aldosterone and synthesis of cholecalciferol.

Unit-IV Natural Plant Pigments and Porphyrins (16 Contact hours)

Introduction, classification, physical, chemical, degradative and spectral methods of structure determination and biosynthesis (Acetate and Shikimic acid pathway)

Flavonoids: Isolation, separation and quantification. Antioxidant activity of flavonoids. Robinson's synthesis, Baker Venketraman synthesis, Kostanecki synthesis of flavanone and Flavanol.

Isolation, structure determination and synthesis of Cyanidin, Chrysin, Quercitin & Genestein.

Porphyrins: Structure determination and total synthesis of haemoglobin. Structural comparison with chlorophyll.

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. New Trends in Natural Product Chemistry, Atta-ur-Rahman (Harward Academic Press).
4. Chemistry of Natural Products, N.R. Krishnaswamy (University Press-1999).
5. Flavanoids; Oyvind M. Andersen and Kenneth R. Markhan. (Taylor & Francis -2006)

Course No: CH17406CR
Title: Bio-Organic and Medicinal Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

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

Vitamins:_ Source, structure and synthesis of vitamins – Vitamin A, Vitamin B-Complex (Thiamine riboflavin, folic acid); Vitamin B-12 (Structure only) Vitamin C, E, K, H and D.

Prostaglandins : Introduction and nomenclature, approaches to prostaglandin synthesis, cyclo-hexane, precursors-Woodward synthesis of PGF2a. Cyclo-heptane precursors - Corey's synthesis of prostoglandin's E & F.Their relationship with oxygenase I and II.

Nucleic Acids: Structure of nucleotide, nucleosides, RNA and DNA, role of nucleic acids in protein synthesis, genetic code and heredity. DNA finger printing

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

Enzymes : Introduction, nomenclature & classification.. Activation & inhibhion of enzymes. Mechanism of enzyme action- Fischer lock and key, koshlands induced fit hypothesis, displacement reactions & coupling of ATP. Enzyme mechanism of chymotrypsin lysozyme & carboxypeptidase.

Co-Enzymes: Cofactors derived from vitamins, coenzymes, prosthetic groups. Apoenzyme. Structure , biological function and mechanism of reactions catalsed by co-enzymes: coenzyme A, thiamine pyrophosphate. pyridoxal phosphate, NAD+, NADP+, FMN, FAD and Lipoic acid.

Unit-III **(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, carbonylic, thiols sulphides groups and introdction/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. Lipophillic constant, Hamett constant, steric parameters and Hansch analysis.

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

Antibiotics: Classifications-structural and mechanistic, cell wall biosynthesis inhibitors, protein synthesis inhibitors. Pencillins-classification and structures. Synthesis of Pencillins, V, G, chloroamphenicol.and ciprofloxacin. Tetracyclins.

Psychoactive Drugs: Introduction, CNS depressants, CNS stimulants, sedatives and hypnotics, barbutirates. Synthesis of diazepam, phenytoins and glutethisimide.

Anti-neoplastic drug: Introduction; cancer chemotherapy, carcenoolytic antibiotic, plant derived anti-cancer agents (Taxol)role of alkylative agents and antimetabolites in treatment of cancer, mitotic inhibitors (elementary idea).

Cardiovascular Drugs: Introduction, cardiovascular diseases, synthesis of Amylnitrate. sorbitrate, quinidine, verapanil, methyl dopa and atenolol

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, Biotechonolgy and Clinical Chemistry of Enzmyes. Trevor Palmer (EWP)
5. Organic Chemistry by I.L.Finar Vol. II (ELBS Longamnn)
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. Chemsitry of Natural Products. S.V. Bhat, B.A. Nagasampagi, M. Siva Kumar. Naroosa Publishing House, New Delhi.

Course No: CH17407CR
Title: Advanced Quantum Chemistry (04 Credits)

Max. Marks: *100* — ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Electronic Structure Theory, Hartree-Fock Method (16 Contact hours)

Review: Electronic Hamiltonian, antisymmetrized wave function, Slater determinant. Hartree-Fock self-consistent field method. One and two-electron integrals in the light of minimal basis H_2 system.

Hartree-Fock Equation, Fock, Coulomb and exchange operators and integrals, restricted Hartree-Fock formalism, Roothaan equation. The Fock matrix elements, Koopman's theorem, Slater-Condon rules. Matrix form of Roothaan equation, the SCF procedure.

Basis Sets: Slatter-type orbitals, Gaussian basis sets. Model SCF calculations on H_2 /$HeH^{+.}$

Unit-II Configuration Interaction and Semiempirical methods (16 Contact hours)

Configuration Interaction: Electron correlation, configuration state functions, configuration interaction (CI), Brillouin theorem, full and truncated CI theories- CID, CISD, CISDTQ methods; Size consistency problem. Moller-Plesset and Coupled Cluster methods.

Semiempirical methods: The ZDO approximation; the PPP method, brief idea of CNDO, INDO and NDDO methods. The MINDO, MNDO, AM1 and PM3 methods.

Unit-III Density Functional Methods and Molecular Properties (16 Contact hours)

Density Functional Theory:Electron probability density. Hohenberg-Kohn theorems, Kohn-Sham formulation of DFT, n- and v- representabilities, E_x&$E_c$functionals; the local density and local spin density approximations, gradient corrected and hybridfunctionals.
Brief idea of Molecular mechanics methods, force fields.

Molecular Properties*:* Potential energy surfaces; molecular geometry and its optimization, Hessian Matrix and normal modes, vibrational frequencies, thermodynamic properties. Dipole moments, atomic Charges.

Unit-IV Use of Quantum Chemistry Software: Gaussian (16 Contact hours)

A quick tour of GAUSSIAN Interface. Input to Gaussian. Model calculations illustrating various features of the package**..**

1. A single point energy calculation: HCHO /CH3.CHO,HCHOMOs.
2. Geometry Optimization: Input and Output for ethene, fluoroethene, propene conformers
3. Transition state optimization $CH_2O \rightarrow HCOH$
4. NMR properties of ethane, ethene and ethyne.
5. Frequency Calculations: Input, Formaldehyde frequencies, Normal modes, zero point energy, thermodynamic properties, polarizability, hyperpolarazability.
6. Stationary points characterization –C3H5F
7. Model Chemistries: Basis set effect on HF bond length

8. Selecting an appropriate theoretical method:
    a) Electron correlation and post SCF methods, limitations of Hartree-Fock theory: HF bond energy, Optimization of O_3.
    b) Density Functional Theory: CO_2 structure and atomization energy.
    c) Butane / Isobutane isomerization energy, rotational barrier in n-butane.

9. Chemical reactions and reactivity:
    a) Hydration enthalpy of the reaction $H^+ + H_2O \rightarrow H_3O^+$
    b) Potential energy surfaces. Reaction path following (IRC calculation) $CH_2O \rightarrow HCOH$
    c) Heat of formation of CO_2 via an isodesmic reaction
10. Solvation models: Formaldehyde Frequencies in Acetonitrile

Books Recommended

1. Quantum Chemistry, Ira. N. Levine, (Prentice Hall, 2009).
2. Quantum Chemistry, 2nd Edn , D. A. McQuarrie, (University Science Books, 2007).
3. Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedmann, (Oxford, 2008).
4. Quantum Chemistry and spectroscopy, Engel & Reid, Pearson (2007)
5. Modern Quantum Chemistry - Introduction to Advanced electronic structure theory - A. Szabo & N. S. Ostlund, (Macmillan, 1982, Dover 1996).
6. Molecular Modeling, Principles and Applications, A. R. Leach, Prentice-Hall, 2001
7. Modern Electronic Structure Theory, D. R. Yarkouy (ed). (World Scientific, 1995)
8. Ab Initio Molecular Orbital Theory, by Hehre, Radom, Schleyer and Pople, (Wiley)
9. Density Functional Theory of Atoms and Molecules, R.G. Parr and W. Yang, Oxford(1989).
10. GAUSSIAN Manual, Gaussian Inc
11. Exploring chemistry with electronic structure methods, Foresman J.B., Frisch A., Gaussian Inc

Course No: CH17408CR
Title: Advanced Electrochemistry and Statistical Mechanics (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Instrumental Methods in Electrochemistry (16 Contact hours)

Fundamentals: Electrode potential and its measurement, standard and formal electrode potentials, three electrode measurements, uncompensated resistance.

Overview of electrode Processes: Faradaic and Non-Faradaic processes, factors affecting electrode reaction rate. Mass transfer: Convection, migration, diffusion, Fick's 1st and 2nd law of diffusion,

Electrochemical Techniques:

Electrophoresis: Factors affecting ion migration, electro-osmosis, theory and applications of capillary electrophoresis.

Potential Step Methods: Chronoamperometry, Chronocoulometry at macro electrodes; theory and applications. Cottrell equation. Controlled-Potential coulometry, Constant-Current coulometric titrations.

Potential Sweep Methods: Linear sweep Voltammetry and Cyclic Voltammetry at macro electrodes theory and applications, Diagnostic criteria of Cyclic Voltammetry.

Unit-II Applied Electrochemistry (16Contacthours)

Electrochemistry of redox enzymes: Direct and mediated electron transfer, Enzyme modified electrodes-challenges and applications. Mechanism and approach to bioelectrosynthesis, examples of bioelectro synthesis-oxidation of alcohols, synthesis of dihydroxy acetone phosphate, site specific oxidation of sugars, reduction of carbonyl compounds, hydrogenation.

Energy storage devices: Desirable characteristics of energy storage devices, Discharge plot, Ragone plot. Batteries: Measures of battery performance. Classical batteries (Lead Acid, Nickel-Cadmium, Zinc-Mangenese dioxide). Modern batteries (Zinc-Air, Nickel-Metal Hydride, Lithium Ion Batteries), Supercapacitors.

Fuel cells, types of fuel Cells, basic fuel cell operation, kinetics of fuel cell reactions. Alkaline, Phosphoric acid, Polymer Electrolyte membrane and direct MeOH fuel cell, biofuel cells.

Unit-III Classical Statistical Mechanics and Ensemble concept (16 Contact hours)

Equations of Motion; Newton, Lagrange and Hamiltonian. Classical partition function, phase space and the Liouville equation, Kinetic theory of gases, equi-partition of energy, Maxwell's velocity distribution.

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. Statistical Mechanical treatment of imperfect gases. Virial equation of state from grand

partition function, virial coefficients in the classical limit, second and third virial coefficients.

Unit-IV Applied Statistical Mechanics (16 Contact hours)

Quantum Statistics: Fermi-Dirac and Boson-Einstein statistics, Nuclear spin statistics, symmetry and nuclear spin, Ortho and Para nuclear spin states, Ortho and Para Hydrogen and Deuterium, CO.

Application of grand partition function to Boson-Einstein and Fermi-Dirac statistics. Ideal Fermi-Dirac gas: Electrons in metals, Ideal Photon gas: Black body radiation, influence of wavelength for the Planck distribution, Bose-Einstein condensation.

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. Electrochemical Methods Fundamentals and Applications, 2ndEdition, Allen J.Bard, Larry R. Faulkner, John Wiley and Sons, INC.
2. Physical Electrochemistry-Principles, Methods and Applications, Israel Rubinstein (Ed.) Marcel Dekker, Inc. New York.
3. Understanding Voltammetry, 2nd Edition, Imperial College Press.
4. Elements of Molecular and Biomolecular Electrochemistry, Jean-Michel Saveant, Wiley-Interscience.
5. Electrochemistry, 2nd Edition, Carl H. Hamann, Andrew Hammett, Wolf Vielstich,Wiley-VCH.
6. Modern Electrochemistry 2B, 2nd Edition, J. O`M. Bockris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.
7. Statistical Thermodynamics, M. C.Gupta ,(NewAgeInternational,1993).
8. Statistical Thermodynamics-Fundamentals and Applications, N.M. Laurendeau, Cambridge University Press, 2005.
9. Statistical Mechanics, D.A. McQuarrie, (Viva,2003).
10. Introduction to Statistical Thermodynamics, Chandler, (OUP, 1987).
11. Statistical Thermodynamics and Kinetic Theory, C. E. Hecht, (Dover,1990).
12. Statistical Mechanics –Principles and Applications, Hill, Dover, 1987.
13. Statistical Thermodynamics for Chemists, A. Ben-Naim, (Plenum, 1992).
14. An introduction to Statistical Thermodynamics, Hill, (Addison-wesley,1987).

Course No: CH17409CR
Title: Chemistry of Materials (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Surfactant mixtures, Stimuli responsive surfactants and block copolymers (16 Contact hours)

Surfactant-Surfactant Interactions: Mixed micelle formation, mixed monolayer formation, synergism, Clint and Rubingh's models of mixed micelle formation**.** Importance and practical applications of mixed surfactant systems.

Stimuli-Responsive Surfactants: Introduction and applications: Biosurfactants, redox, photochromic, thermoreversible, pH-sensitive, cleavable and magnetic surfactants.

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

Unit-II Hydrogels and microemulsions (16 Contact hours)

Hydrogels: Introduction, Types of Hydrogels, Preparation, Properties and characterization of Hydrogels, Biomedical applications of Hydrogels.

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

Unit-III Langmuir Blodgett Films, Liquid crystals and Fullerenes (16 Contact hours)

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.

Fullerenes: Fullerenes- History, bonding, properties, doped fullerenes, fullerenes as superconductors and fullerene related compounds (carbon nanotubes).

Unit-IV Optical materials and Ionic conductors (16 Contact hours)

Optical materials: Luminesence and phosphors. Lasers – general principle of lasing action, Ruby laser, Neodymium-YAG lasers, semiconducing lasers and quantum dot lasers. Nonlinear optical effects, second and third order harmonic generation, nonlinear optical materials.

Ionic Conductors: Introduction to ionic conduction and mechanism. Types of ionic conductors, mechanism of ionic conduction, interstitial jumps (Frenkel); vacancy

mechanism. Super-ionic conductors: Diffusion and transition superionic conductors and mechanism of conduction in superionic conductors; examples and applications of ionic conductors.

Books Recommended:

1. M. J. Rosen, J. T. Kunjappu, "Surfactants and Interfacial Phenomena", John Wiley & Sons, New York, 4th Edition, 2012.
2. R. D. Vold and M. J. Vold, "Colloid and Interface Chemistry", Addison-wesley, 1982.
3. .D. Y. Meyer, "Surfaces, Interfaces and Colloid", VCH Publishers, Inc. 1991.
4. Jonsson, Lindmann, Homberg and Kronberg, "Surfactants and polymers in aqueous solution", John Wiley and sons, 1998.
5. D. Fennell Evans, H. Wennerstrom, "The Colloidal Domain where physics, chemistry, biology and technology meet" VCH, New York, 1994.
6. Robert J. Hunter, "Foundations of Colloid Science", Oxford University Press, New York, 2007.
7. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
8. I. W. Hamley, The Physics of Block Copolymers (Oxford University Press, Oxford, 1998.
9. N. Hadijichristidis, S. Pispas and G. A. Floudas Block Copolymers (Wiley, New York, 2003).
10. Introduction to Solids, Azaroff, Tata McGraw,1993.
11. SolidState Chemistry and its Applications, West, Wiley,1989.
12. The Physical Chemistry of Solids, Borg, Biens, Academic press, 1992.
13. Solid State Physics, N. W. Ashcroft and N. D. Mermin, Saunders college, 2001
14. Principles of Solid State, H. V. Keer, Wiley Eastern.
15. The Physics and Chemistry of materials, J.I. Gersten, F.W. Smith, John Wiley and sons, Inc. 2001.
16. Microemulsions: Background, New Concepts, Applications, Perspectives, C. Stubenrauch, Blackwell Publishing Ltd, 2009.
17. M. Sirousazar, M. Foroug, K. Farhad, Y. Shaabani and R. Molaei, Hydrogels: Properties, Preparation, Characterization and Biomedical, Applications in Tissue Engineering, Drug, Delivery and Wound Care, IN Advanced Healthcare Materials, Wiley online Library, 2014.

Course No: CH17410DCE

Title: Advanced Laboratory Course in Inorganic Chemistry (04 Credits)

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

External Exam: *75 Marks.* ***Internal Assessment****: 25 Marks*

A: - Inorganic Preparations: (5 Experiments)

- Preparation of tetraamminecarbonatocobalt (III) nitrate and its conversion to pentaamminecholorocobalt (III) chloride.
- Preparation of trans dicholoro bis (ethylenediamine) cobalt (III) chloride and its conversion to cis-isomer.
- Preparation of tris (ethylenediamine) nickel (II) chloride dihydrate and its conversion to bis (ethylenediamine) nickel (II) chloride.
- Preparation of bis (acetylacetonato) copper (II) dihydrate.
- Preparation of pentaamminecholorocobalt (III) chloride and study of Linkage isomers by its conversion to pentaamminenitritocobalt (III) chloride and to nitro isomer followed by IR Characterization.

B:- Total analysis of a Coordination compound for determination of various components present.

(1- Experiment)

C: - Separation by Column Chromatography and Estimations: (5 Experiments)

- Separation of Permanganate and Bichromate ions on Alumina column and their Estimation from Beer Law plots.
- Determination of lonisable chloride in a Complex by cation exchange column (separation followed by Mohr's titration of elute for estimation).
- Separation of Cobalt (II) and Nickel (II) on anion exchange column followed by estimation through EDTA titrations.
- Separation of two Cobalt (III) complexes viz $[Co(NH_3)_6] Cl_3$ and $[Co (NH_3)_5 Cl] Cl_2$ on Silica column.
- Ion exchange separation of Hydration / ionization isomers of Chromium (III) Chloride ($CrCl_3$).

D: - Potentiometric Titrations: (6 Experiments)

- Standardization of an Iron (ii) solution with a standard dichromate solution over Pt & Calomel assembly.
- Determination of purity of Ce (IV) Sulphate with a standard Iron (II) solution over Pt & Calomel assembly.
- Estimation of Iodide with Standard $AgNO_3$ over Pt & Calomel assembly using I^- \ I2 redox couple.
- Simultaneous determinations of Chloride and Iodide ions with Standard $AgNO_3$ over Ag-Glass electrode assembly.
- Determination of the purity of $[Co (NH_3)_5Cl] Cl_2$ over Ag-Glass electrode assembly.
- Complexometric titration for determination of Ferro cyanide with standard Zinc (ii) solution and inorder to establish the composition of the complex $K_2Zn_3[Fe(CN)_6]_2$

E: - pH-metric Titrations: (2 Experiments)

- Quantitative analysis of Chromate Dichromate mixture by pH Titration.
- Purity of Acetyl Salicylic acid (Asprin) in a commercial tablet by pH Titration.

F: - Conductometric Titrations: (2 Experiments)

- To determine the solubility and solubility product of a sparingly soluble salt ($BaSO_4$) in water.
- To determine the basicity of sodium potassium tartarate by Conductometric method.

G:- Spectrophotometry: (5 Experiments)

- Determination of Iron (II) with 1,10-Phenanthroline.
- Determination of Phosphate by Molybdenum blue method.
- Determination of formula of Iron (III) thiocyanate complex by Job's Continuous variation method.
- Determination of composition of Iron (II)—2,2-bipyridyl complex by Mole ratio method.
- Determination of rate of Aquation of complex $[Co(NH_3)_5Cl]Cl_2$ in acidic medium.

H: - Flame Photometry: (2 Experiments)

- Simultaneous determination of Sodium and Potassium in the given mixture.
- Determination of Cadmium and Magnesium in tap water.

Books Recommended:

- Vogel's quantitative analysis 6 Edn. Mendham, Denny; Pearson Education 2002
- Synthesis and Technique in Inorganic chemistry , G. S.Girlomi; R.J. Angleci 3rd edn.; University Science Books.
- Synthesis and characterization of Inorganic compounds W.AJolly
- Inorganic syntheses Vols II, VI Academic Press.
- Experimental Inorganic / Physical Chemistry ; Mounir A. Malati Horwood/1999.
- Quantitative Chemical Analysis ; 5th edn.; Harris ; Freeman ; 1999.
- Advanced Practical Inorganic Chemistry ; Adams ; Raynor, Wiley ; 1995.
- Advanced Experimental Inorganic Chemistry ; Ayodha Singh ; Campus Books 2002.

Course No: CH17411DCE

Title: Advanced Laboratory Course in Organic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *75 Marks.* ***Internal Assessment****: 25 Marks*

1. **Multistep synthesis of drugs/ organic coinpouiuls involving name reactions**
   (1) Synthesis oflocal 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.
2. **Extraction/Estimation of Organic compounds from Natural sources**
   (1) Isolation of lycopene and β-carotene from tomato and their characterization using *uv*- spectroscopy.
   (2) Isolation of limonene from its natural source and physicochemical analysis.
   (3) Assay of Belladona for Hyoscyamine.
   (4) Assay of lemon from citric acid and vitamin-C
   (5) Isolation of cholesterol from gallstone
   (6) Assay of coke (soft drink)
3. **Column Chromatography**
   Separation of two component solid mixture. Identification of separated components using physical, chemical and spectral techniques.
4. **Spcctrophotomctric estimation** (UV/visible)
   (1) Vitamin-C (Ascorbic acid)
   (2) Caffeine from tea.
   (3) Cholesterol
   (4) Aspirin
5. **Elcctrophoresis/ Paper chromatography**
   Separation and identification of aminoacids by elcctrophoresis / Paper chromatography.
6. **Spcctroscopy**
   Identification of Organic compounds through interpretation of their spectra (UV, IR, PMR, CMR and Mass. Spectra to be provided).

Books Recommended :

1. Comprehensive Practical Organic Chemistry, V.K. Ahluwalia, Renu Aggarwal (Univ. Press India Limited -2000).
2. Vogel's Text Book of Practical Organic Chemistry, B.S.Furniss, A. J. Hannaford (AWL 5^{th} Ed.-1998).
3. Organic Laboratory Techniques , Donald .C. Pavia, Gary . M. Lampman (SCP 3rdEd.-1999)
4. Experiment Organic Chemistry, John.C. Gilbert., Stephen.F.Martin (SCP -1998)
5. Advanced Practical Organic Chemistry Vol. II, Jag Mohan (Himalaya Pub. House First Ed.-1992.

Course No: CH17412DCE
Title: Advanced Laboratory Course in Physical Chemistry (04 Credits)

Max. Marks: *100* — ***Duration:*** *64 Contact hours*
External Exam: *75 Marks.* — ***Internal Assessment****: 25 Marks*

A. Tensiometry

1. Investigation of variation of surface tension of n-butanol and sodium chloride solutions with concentration and hence determination of their surface excess concentrations using Gibb's Adsorption Isotherm.
2. Determination of CMC value of a detergent using tensiometry.

B. Cryoscopy

1. Investigation of variation of freezing point depression with concentration & determination of molecular mass.
2. Determination of the degree of dissociation of a salt/weak acid in solution.
3. Determination of activity co-efficient from freezing point measurements.

C. Spectrophotometry

1. To study the complexation reaction between Fe(III) & salicylic acid.
2. Determination of pK value of an indicator.

D. Spectrofluorometry

1. To determine the rate constant for fluorescence quenching of anthracene or perylene by CCl_4 in ethanol.
2. Using pyrene as probe determine the cmc of a surfactant and site of solubilization of pyrene in the micelle through spectrofluorometry.

E. Potentiometry

1. Precipitation titration of KCl, KBr, KI and their mixture with $AgNO_3$
2. Thermodynamics of a chemical reaction by EMF-method.
3. Determination of (a) Standard electrode potential & (b) Activity Coefficient.

F. Conductometry

1. Verification of Debye-Huckel-Onsagar law.
2. Precipitation titration of $BaCl_2$ and K_2SO_4/ $(NH_4)_2SO_4$
3. Estimation of the concentrations of H_2SO_4, CH_3COOH and $CuSO_4$ in a mixture.

G. Dynamic Electrochemistry

1. To estimate the surface area of a working electrode through chronoamperometry and chronocoulometry.
2. Using Cyclic Voltammetry to determine the formal potential and diffusion coefficient of $[Fe(CN)_6]^{3-}$.
3. Use cyclic voltammetry to determine the concentration of acetaminophen in a given sample.

H. Kinetics

1. Kinetic Investigation of BZ-Oscillatory reaction.
2. Kinetic study of enzyme catalyzed reaction (effect of pH and Temperature).

I. Viscometry and densitometery

1. Determination of Mol. Mass of a Polymer (Polyv inyl alcohol) using viscosity method.
2. To explore the nature of chemical bonding (head-head and Head tail linkage of monomers) in polyvinyl alcohol using Viscometry.
3. Determination of partial molar volume of sodium chloride solutions as a function of concentration from density measurements.

Books Recommended

1. Practical Physical Chemistry --- Findley revised by Kitchner.(Longman, 1971)
2. Experimental Physical Chemistry, A. M. Halpern, G. C. McBane, (Freeman, 2006)
3. Experiments in Physical Chemistry, 5th ed. --- Schoemaker et al. (MGH, 2003)
4. Experimental Electrochemistry---R. Holze (Wiley-VCH, 2009).

Course No: CH17413DCE

Title: Supramolecular Chemistry (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*

Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Supramolecular Interactions (08 Contact hours)

Definition and Development of Supramoleclar Chemistry. Nature of Supramolecular Interactions.

Hard Soft Acid Base Concept- Concept, Classification, Symbiosis. Utility in drug design and molecular recognition. Soft Ligands for Soft Metal Ions-Mixed Crown Ethers and Mixed Cryptands.

Unit-II Supramolecular Receptors (08 Contact hours)

Cation Receptors: Supramolecular Cation Coordination Chemistry, EDTA- The Supramolecular Host. Introductory account of Cation Receptors - Podands, Corands, Cryptands, Spherands and Calixarenes.

Anion Receptors: Scope and Challenges, Anion Hydrophobicity-Hofmeister Series, Introductory Account of Anion Receptors - Cyclophanes, Pyrolles, Azacrowns and Metal Based receptors. Hydride Sponge and Anticrowns.

Ion-Pair Receptors: Concept and Significance

Unit-III Crystal engineering and Supramolecular Motiffs (08 Contact hours)

Crystal Engineering: Introduction, Tectons and Synthons. Hydrogen Bond- Introduction, Criteria

Nature and Importance.

Self Assembly: Scope and Objectives. Concepts and Classification. Introductory Account of Coordination Capsules, Catenenes, Rotaxenes and Molecular Knots.

Unit-IV Network Solids and Molecular Devices (08 Contact hours)

Network Solids: Concepts and Classification, Network Topology. Zeolites: Structure, utility and limitations. Metal Organic Frameworks-Introduction and application in catalysis and Gas storage.

Molecular Devices**:** Philosophy of Molecular Devices, Photophysical Fundamentals and Mechanism of Energy and Electron Transfer, Introductory Account of Molecular Wires, Molecular Switches and Molecular Motors.

Books 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, Ist 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. Chemical Reviews. Vol. 115, Issue 15, year **2015**, Pages 6999-8156
8. Introduction: Supramolecular Chemistry. F. Huang and E. V. Anslyn. Chem. Rev. **2015**, 115, 6999−7000.
9. Supramolecular materials. D. B. Amabilino, D. K. Smith and J. W. Steed. Chem. Soc. Rev., **2017**, 46, 2404—2420
10. A Bond by Other Name. G. R. Desiraju. Angew. Chem. Int. Ed. **2011**, 50, 52-59.
11. The Weak Hydrogen Bond: In Structural Chemistry and Biology. G. Desiraju, T. Steiner. **Oxford, IUCr Monograph on Crystallography**.

Course No: CH17414DCE
Title: Designing Organic Synthesis (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I (A) Oxidative and Reductive Processes in Organic Synthesis (8 Contact hours)

***Oxidation*:** Introduction, Aromatisation of cycloalkanes and alkenes using metal catalysts and DDQ. Oxidation of Alcohols using chromic acid, DCC and Swern reagent. Oppenaur oxidation. Oxidation of ketones. Oxidation at activated carbon-hydrogen bond. Oxidation with Selenium dioxide. Prevost hydroxylation and its modification by Woodward.

***Reduction*:** lntroduction. Reduction of Alkenes, Alkynes and Aromatic rings.

Reduction of carbonyl compounds: Clemmensen and Wolf-Kishner reductions. Reductions using $LiAlH_4$ and $NaBH_4$ Bouveault-Blanc reduction. Reduction of Epoxides, Nitro, Nitroso, Azo and Oxime groups. Reductions using Tributyl Tin Hydride.

(B) Protection and Interconversion of Functional Groups (8 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-II 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, α, β-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; Verlage VCH;1986.
3. Principles of Organic Synthesis 2nd edn;. R. O. C. Norman; Chapman and Hall; 1978.
4. Advanced Organic Chemistry Part B, 5th edn.; F. A. Carey and R.J Sundberg ; Springer; 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, 6lh Ed., J. March,; Wiley; 2012.
9. Organic Synthesis- The disconnection Approach; Sturat Warren; Wiley; 2013

Course No: CH17415DCE
Title: Computational Chemistry (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I

(a) Numerical solution of equations (8 Contact hours)

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

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

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

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

(b) Numerical differentiation and integration (8 Contact hours)

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

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

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

Unit-II

(a) Interpolation and Curve Fitting (8 Contact hours)

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

Lagrange's interpolation method, Newton's divided differences, Cubic spline, piece wise interpolation.

Least squares approximation, linear and quadratic.

(b) Use of Mathematica/Scilab for numerical solution of problems(8 Contact hours)

The mathematica package will be used for the solution of problems covered under the above three units.

Books Recommended

1. Data Reduction & Error Analysis, Bevington& Robinson, (McGraw-Hill, 2003)
2. Computational Chemistry, A. C. Norris, (Wiley.)
3. Computer Software Applications in Chemistry - P. C. Jurs, (John Wiley, 1996.)
4. Numerical Methods for Scientists and Engineers, H. M. Antie, (TMH,).
5. Numerical Recipes in Fortran/C, W.H. Press et al., (CUP,1992)
6. Applied Numerical Analysis, Gerald &Wheatly, (Pearson Education, 2002)
7. Mathematical Methods for Scientists and Engineers, D.A. McQuarie, Viva Books, 1st Ed., 2009.
8. Mathematica Manual.

Course No: CH17416DCE
Title: Seminar (02 Credits)

Presentation by a candidate on any topic chosen in consultation with the teacher incharge.

(25 Marks)

Manuscript (on the topic) submission (25 Marks)

Course No: CH17417GE
Title: Synthetic Polymers and their Applications (02 Credits)

Max. Marks: *50* — ***Duration:*** *32 Contact hours*

Ist Unit Exam: *25 marks* — ***IInd Unit (Term end) Exam:*** *25 marks*

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

Course No: CH17418GE
Title: Novel Materials (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

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

Block Copolymers: Introduction: classification, micellization of diblock 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, photoconductivity and sensors.

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

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

Luminesence and phosphors. Lasers - general principle of lasing action, Ruby laser, semiconducing 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 Nanofluids 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, Jeremy Ramsden and Ventus Publishing ApS, 2009.

Course No: CH17419OE
Title: Food Chemistry (02 Credits)

Max. Marks: *50* — ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit (Term end) Exam:*** *25 marks*

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_2, 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; 3rd Ed.; Marcel Dekker, Inc. NY; 2005.
2. Food: The Chemistry of its components; T.P. Coultate; 3rd 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; 2nd ed.; Springer International Edition; 2005.

Course No: CH17101CR
Title: Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Stereochemistry and Bonding in the Compounds of Main Group Elements (16 Contact hours)

Valence bond theory: Energy changes taking place during the formation of diatomic molecules; factors affecting the combined wave function. Bent's rule and energetics of hybridization.

Resonance: Conditions, resonance energy and examples of some inorganic molecules/ions.

Odd Electron Bonds: Types, properties and molecular orbital treatment.

VSEPR: Recapitulation of assumptions, shapes of trigonal bypyramidal, octahedral and pentagonal bipyramidal molecules / ions. (PCl_5, VO_3^-, SF_6, $[SiF_6]^{2-}$, $[PbCl_6]^{2-}$ and IF_7). Limitations of VSEPR theory.

Molecular orbital theory: Salient features, variation of electron density with internuclear distance. Relative order of energy levels and molecular orbital diagrams of some heterodiatomic molecules /ions. Molecular orbital diagram of polyatomic molecules / ions.

Delocalized Molecular Orbitals: Butadiene, cyclopentadiene and benzene.

Detection of Hydrogen Bond: UV-VIS, IR and X-ray. Importance of hydrogen bonding.

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

Stepwise and overall formation constants. Inert & labile complexes. Stability of uncommon oxidation states.

Metal Chelates: Characteristics, Chelate effect and the factors affecting stability of metal chelates.

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-III Bonding 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 ML6; Effect of pi-bonding. Molecular orbital and energy level diagram for bonding in Ferrocene, Square-planar and Tetrahedral complexes.

Unit-IV Pi-acid Metal Complexes (16 Contact hours)

Transition Metal Carbonyls: Carbon monoxide as ligand, synthesis, reactions, structures and bonding of mono- and poly-nuclear carbonyls. Vibrational spectra of metal carbonyls for structural diagnosis.

Prepration, reactions, structure and bonding of transition metal nitrosyls, dinitrogen and dioxygen complexes.

Tertiary phosphine as ligand.

Books Recommended

1. Principles of Inorganic Chemistry; 1st edn.; Brain W. Pfennig; Wiley; 2015.
2. Advanced Inorganic Chemistry; 5th. and 6th edn; F.A. Cotton , G. Wilkinson; Wiley; 1998/1999.
3. Inorganic Chemistry; 4th edn; J. E. Huheey; E. A. Keiter; Harper Collins; 2009.
4. Inorganic Chemistry; G. Wulfsberg; Viva; 2002.
5. Chemistry of the Elements; 2nd edn; N. N. Greenwood, A. Earnshaw; Butterworth; 1997.
6. Inorganic Chemistry; 3rd edn; D. F. Shriver; P. W. Atkins; Oxford; 1999.
7. Inorganic Chemistry; K.F. Purcell, J.C Kotz; Saunders; 1977.
8. Coordination Chemistry; D. Banerjea; Tata McGraw Hill; 1993.

Course No: CH17102CR
Title: Organic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Delocalized Chemical bonding (16 Contact hours)

Overview: Inductive effect. Conjugation, Cross conjugation, Hyperconjugation–Isovalent and sacrificial hyperconjugations, Acids / Bases, Nucleophiles and Electrophiles. Resonance, Rules for writing resonance structures, Steric inhibition of resonance.

Tautomerism: Different types including valence 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.

Unit-II Reactive Intermediates and Determination of Reaction Mechanism (16 Contact hours)

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

Determination of Reaction Mechanism: Reaction Mechanism & Types of reactions. Determining reaction mechanism: Structure of Product, Transition states & Intermediates (Hammond postulate). Catalysis including acid and base catalysis, Specific acid and base catalysis. Fate of individual atoms (Isotope Labeling). Stereochemical course of reaction. Thermodynamic and kinetic evidences. Correlation of structure – reactivity.

Unit-III Stereochemistry: (16 Contact hours)

Chirality: Introduction, Chirality due to chiral centre. Molecules with more than one Chiral centres, Threo and erythro isomers. Convention for of assigning D, L & R, S configurations. Optical activity due to chiral axis, chiral plane and helicity. Chirality involving atoms other than carbon. Chirality in metallic complexes. Enantiotopic and diastereotopic atoms, groups and faces.

Asymmetric Synthesis: Introduction and principle of asymmetric synthesism. Principal categories of asymmetric synthesis. Use of chiral substrates. Diastero-selectivity in Aldol reactions. Sterospecificity and steroselectivity of enzymes.

Confirmations: Origin of conformational energy. Angle and Pitzer strain. Conformational analysis of cycloalkanes, and decalines. Effect of conformation on reactivity in acyclic and cyclic systems. Conformation of sugars & anomeric effect. Conformation of cyclohexene, cyclohexanones and bicycloheptane – a bridged system.

Unit-IV Aliphatic Nucleophilic Substitutions : (16 Contact hours)

Mechanism and stereochemical implications of S_N2, S_N1, S_Ni and Neighbouring Group Participation (by π and σ-bonds) reactions. Comparison of S_N1 and S_N2 reactions. Effect of substrate structure, attacking nucleophile, leaving group and solvent on the rates of S_N1 and S_N2 reactions. Mixed S_N1 and S_N2 reactions. Nucleophilic substitution at allylic, benzylic, aliphatic trigonal and vinylic carbons. Nucleophilic substitution in alcohols, Mitsunobu reactions. Nucleophilic substitutions on other elements. Functional group transformation using S_N2 reactions in organic synthesis. Nucleophilic substitutions in biological systems.

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

Aliphatic Electrophilic Substitutions: General mechanism of S_E1, S_E2 and S_Ei reactions. Mechanisms of reactions involving migration of double bond. Effect of substrate, leaving group and solvent on reactivity. Stork-Enamine reaction.

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 3rd Ed., S.M. Mukherjee and S.P. Singh. (Macmillan-1998).
4. Stereochemistry of Organic Compounds 2nd Ed., D. Nasipuri. (New Age Inter.- 2008)
5. Stereochemistry of Carbon Compounds - E.L.Eliel. (TMH -2007)
6. Stereochemistry of Organic Compounds 7th Ed. - P.S. Kalsi. (New Age Inter.- 2012).
7. Organic Chemistry - 2nd Ed., J. Hornback. (Brooks/Cole- 2006,
8. Organic Chemistry, 5th Ed., John McMurry. (Brooks/Cole-2000).
9. Advanced Organic Chemistry, 5th Ed., F.A Carey & R.J Sundberg (Springer-2007).
10. Organic Chemistry, 2nd Ed., Jonathan Clayden (OUP-2012)
11. Organic Chemistry, 11th Ed., Solomons, T.W.G., (Wiley-2015).

Course No: CH17103CR
Title: Physical Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

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)

Theories of Chemical Reactions: Activated complex theory of reaction rates, statistical & thermodynamic formulations, comparison with collision theory. Theories of unimolecular reactions (Lindman, Hinshelwood , RRK and RRKM theories), Introduction to potential energy surfaces.

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

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

Unit-IV Chemical kinetics-II **(16 Contact hours)**

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

Reactions in solutions: Diffusion controlled reactions (partial & full microscopic diffusion control), Ionic Reactions; Single & double sphere models of ionic reactions.

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

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

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. CH17104DCE

Title: Laboratory Course in Inorganic Chemistry (04 Credits)

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

External Exam: *75 Marks.* ***Internal Assessment****: 25 Marks*

I. Preparation of Coordination compounds of Transition metals:

1. Theoretical appraise of first row Transition metal Coordination Chemistry.
2. Synthesis as a Laboratory Technique (Concepts, Calculations and Design of Synthetic procedures).
3. Selected preparations of the following coordination compounds with the specific objectives:

i) Mercurytetrathiocyanatocobaltate(II)	:	To visualize the complexation process.
ii) Tristhioureacopper(I)sulphate monohydrate	:	Insitu generation and Stabilization of unusual oxidation state and re-crystallization /crystal growing
iii) Hexaamminecobalt(III) chloride	:	Multistep synthetic procedure
iv) Trisethylenediaminecobalt(III) chloride	:	Two stage synthesis and aerial oxidation/Resolution of a racemic mixture
v) Ammonium dodeca molbedophosphate	:	Synthesis of a heteroploy metallate/ Bonding and structure.

II. 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.

III.

A. Qualitative Analysis by Semi micro Technique:

Discussion about the analysis scheme. Analytical groups and Group reagents. Scales of Analysis, Skill of semi micro technique. Chemistry involved in separation and identification of less familiar cations by semi micro analysis.

B. Identification of four less familiar cations from different analytical groups with simple and complex combinations:

(i) Group I and II A

(ii) Group I, II A and II B

(iii) Group IIA and II B

(iv) Group I and Group III

(v) Group II B and Group III

(vi) Group III only.

IV. Inorganic Quantitative Analyses:

A. **Gravimetry:**

i) Skill and importance of weighing in Chemistry, Gravimetreric 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.

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) Barium (Ba^{2+}) as BaSO4 and Zinc as $[ZnEDTA]^{2-}$ complex.

iii) Barium (Ba^{2+}) as $BaSO_4$ and Nickel (Ni^{2+}) as $[NiEDTA]^{2-}$ complex.

iv) Nickel (Ni^{2+}) as Ni $(dmg)_2$ complex and Magnesium (Mg^{2+}) as $[Mg\ EDTA]^{2-}$ complex.

v) Copper (Cu^{2+}) as CuSCN and Magnesium (Mg^{2+}) as $[MgEDTA]^{2-}$ complex.

Books Recommended:

1. Advanced Inorganic Chemistry, 5th ed. / 6th 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; 5th edn; Jeffery, Bassett; (ELBS, 1989).
4. Quantitative Analysis; 6th edn; Day, Underwood (Printice Hall, 1993).
5. Analytical Chemistry, 6th Ed; D. Christian, Wiley.
6. Quantitative Analysis; 6th edn; Day, Underwood (Printice Hall, 1993).

Course No: CH17105DCE
Title: Symmetry and Group Theory (02 Credits)

***Max. Marks:** 50* | ***Duration:** 32 Contact hours*
***Ist Unit Exam:** 25 marks* | ***IInd Unit (Term end) Exam:** 25 marks*

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, Symmetry groups and group multiplication tables.

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 Orthoganality Theorm-elementary idea, consequences of the Great Orthogonolity Theorem. Reducible and Irreducible representations, Mullikan symbols for IRS. Character table-construction of character tables for C2v, C3v and C4v point groups.

Applications of group theory to IR and Raman spectroscopy, 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 and Polarity.

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.

Course No: CH17106DCE
Title: Infrared, Raman and Electronic Spectroscopy (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

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_2, O_2),

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. Physical Methods for Chemists; R.S.Drago; 2nd edn; Saunders; 1992.
2. Fundamentals of Molecular Spectrsocopy; C.N.Banwell, E.M.Mc Cash; 4th edn; Tata McGrawHill; 1994.
3. Physical chemistry; P. W. Atkins; 6th edition; Oxford University Press; 1998.
4. Electronic Absorption Spectroscopy and related techniques; D N Sathyanarayna; UniversitiesPress.
5. Introductory Raman Spectroscopy; J. R. Ferraro, K. Nakamoto & C. W Brown; 2nd edn; Academic Press 2005.
6. Theory and Applications of Ultraviolet Spectroscopy; H.H.Jaffe, M.Orchin; Wiley; 1962.
7. Molecular Spectroscopy; 1st edn; J L. McHale; Prentice Hall; 1999.
8. Modern Spectroscopy; J.M.Hollas; Wiley; 1987.
9. Basic Principles of Spectroscopy; R.Chang; McGraw Hill; 1971.
10. Structural Methods in Inorganic Chemistry; 2nd edn; E.A.V.Ebsworth, D.W.H.Rankin, S.Cradock; Blackwell; 1991.

Course No: CH17001GE

Title: Chemistry of the Environment (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*

Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Soil and Hydrosphere (16 Contact hours)

Soil: Nature and Composition of soil – Air, Water, Inorganic components, organic matter and humus. Acid – Base and Ion exchange reactions in soil.

Wastes and pollutants in soil: Chemical degradation, photochemical reactions and biodegradation. Desertification, Deforestation and soil erosion.

Hydrosphere: Chemical Composition of Water Bodies: Lakes & rivers, Factors determining composition (thermal stratification, acid-base, pE concept).

Aquatic pollution: Inorganic, Organic, Pesticide, Agricultural, Industrial and Sewage.

Water quality parameters: Dissolved oxygen, Metals, Content of Chloride, Phosphate, Nitrate, and Microorganisms. Water quality standards.

Analytical Methods for determining BOD, DO, COD, and choice of methods for determining metals (As, Cd, Hg, Pb & Se).

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

Unit-II Atmosphere (16 Contact hours)

Chemical Composition of the Atmosphere: Particles, ions, radicals and their formation. Vertical profile of the atmosphere, Heat budget of earth's atmospheric system. Chemical and photochemical reactions in atmosphere, photochemical smog formation.

Oxides of N, C, S and their effects.

Ozone layer: Formation of ozone and mechanism of ozone depletion.

Pollution by chemicals: Chlorofluorocarbons, hydrocarbons and ozone.

Green house effect: Cause, source and impact on global climate.

Consequences of Green house effect and remedial measures.

Acid rain: Chemical aspects, adverse effects and control.

Books Recommended

1. Environmental Chemistry; 5th edn; Colin Baird; Freeman & Co; 2012.
2. Environmental Chemistry; 9th edn.S.E.Manahan; Lewis Publishers;2009
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 pollution; B.K.Sharma & H.Kaur; Goel Publishcrs;1996.
7. Environmental Chemistry; Nigel. J.Bunce; Wurez Publishers; 1991.
8. Environmental Toxicology; Ed.Rose; Gordon & Breach Science Publishers.

Course No: CH17002GE
Title: Surfactants and their Applications (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Self-Assembly of Surfactants (16 Contact hours)

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 Systems (16 Contact hours)

a) **Mixed Surfactant systems**: Mixed micelle formation, mixed monolayer formation, synergism, various models of mixed micelle formation(Clint, Rubingh, Motamurra, Blankschtein, and Rubing-Holland models) 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. Characterization of polymer- surfactant systems by various techniques like viscosity, light scattering, spectroscopic and conductance measurements. 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. Physical Chemistry; P.W. Atkins; ELBS; Oxford; 1994.
3. Principles of Colloid and Surface Chemistry; P.C. Heimenz; Marcel Dekker Inc; New York; 1986.
4. Surfactants and Interfacial Phenomena; M. J. Rosen; John Wiley & Sons; New York; 1989.
5. Colloid and Interface Chemistry; R. D. Vold and M. J. Vold; Addison-Wesley; 1982.
6. Surfaces, Interfaces and Colloid; D. Y. Meyer; VCH Publishers; Inc; 1991.
7. Surfactants and polymers in aqueous solution; Jonsson, Lindmann, Homberg and Kronberg; John Wiley and sons; 1998.
8. Advances in Colloid and Polymer Science; B.K.Paul & S.P.Moulik, Current Science,Vol.80,p 990-,2001; Vol.78,p 99,1998.
9. Critical Reviews in Food Science and Nutrition; John Flanagan & Harjinder Singh, ,Vol. 46, pp221-237, 2006.
10. Advanced Drug Delivery Reviews; M. J. Lawrence & G.D.Rees; Vol, 45, p 898, 2000.
11. Energy Fuels; T. N. Dantas, A.A.D, Netoetal; DOI:10.1021/ ef900952y; 2010.

Course No: CH17001OE
Title: Chemistry in Everyday Life (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

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

(a) Water- An Amazing Chemical Stuff

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)

Course No: CH17201CR
Title: Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

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

Energy profile of a reaction; reactivity of metal complexes; inert and labile complexes.
Types of substitution reactions; mechanistic classification of substitution reactions:- Dissociative, Associative, Dissociative conjugate base and Interchange.
Empirical criteria to differentiate the mechanism of substitution reaction.
Substitution in octahedral complexes- Classification of metal ions based on water exchange rates. Metal-complex formation- the Eigen-Wilkins mechanism. Anation reactions.
Hydrolysis Reactions; Simple Acid hydrolysis, Acid catalysed and Base hydrolysis. Stereochemical changes in Octahedral Substitution Reactions.
Substitution reactions without breaking of metal-ligand bond.

Unit-III Mechanism of Ligand Substitution Reactions in Square-Planar complexes:
(16 Contact hours)

Significance of the two-term rate^law, Mechanism, and Steric course of the substitution reactions.
Factors affecting the rate of substitution:- entering and leaving groups; nucleophilicity of entering group and the n_{pt} scale, central metal ion, solvent and the non-leaving groups.
The Trans effect;- Theories, applications in synthesis.
cis-trans isomerization in square planar complexes.

Unit-IV Organo Metallic Compounds (16 Contact hours)

Introduction, Nomenclature, classification and importance of organometallic compounds.
Nomenclature and Classification of Organometallic compounds.
Effective atomic number (18-Valance electron) rule and its significance.
Stability of Organometallic Compounds towards heat, oxidation and hydrolysis.
Preparation, Properties, Structure, bonding and applications of Alkyls and aryls of Li, B and Al.
Synthesis, Structure and bonding in Zeise's Salt.
Homogenous Catalysis using Organometallic Compounds: Catalysis, Terminology of Catalysis and Tolman Catalytic loop;
Oxidative addition, reductive elimination and migration (insertion) reactions.
Hydrogenation and Hydroformation reactions in alkenes.

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. CH17202CR
Title: Organic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Aromatic Electrophilic Substitution (16 Contact hours)

Overview: Arenium ion mechanism, Sigma and pi – complexes, Energy profile diagram, Effect of leaving group. Orientation and reactivity in mono substituted benzene ring , *Ortho / Para ratio*, Ipso attack.

The Third substitution : Orientation of substitution in benzene ring with more than one substituent. Orientation in other ring systems. Carboxylation of aromatic rings with $COCl_2$ and amidation with NH_2COCl. Reversal of F.C. acylations. 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 mechanism (S_N1, S_NAr, Benzyne and $S_{RN}1$). Structure reactivity relationships. Effect of leaving group and attacking nucleophile. Mechanisms of Von-Richter, Sommelet-Hauser and Smiles rearrangements and Chichibabin reaction.

Free Radical Substitution:

Free radical substitution mechanisms. Mechanisms at an aromatic substrate. Neighbouring Group Assistance in free radical reactions, Reactivity for aliphatic and aromatic substrates. Reactivity in the attacking radical. Effect of solvent on reactivity.

Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sandmeyer reaction, free radical rearrangements and Hunsdiecker reaction.

Unit-II Addition to multiple bonds. (16 Contact hours)

Addition to carbon-oxygen double bonds:

Overview of reactivity carbonyl compounds: Mechanisms of addition of water , hydrogen cyanide, alcohols , amines , organometallic reagents and hydrides to aldehydes and ketones.

Mechanism of Wittig, Mannich , Aldol, Cross Aldol , Cannizarro's , Knoevenagel, Robinson annulation, Claisen, Dickman , Benzoin , Perkin and Stobbes reactions.

Addition to carbon-carbon multiple bonds:

General mechanism, reactivity, orientation and stereochemical implications of additions reactions involving electrophiles, nucleophiles and free radicals. Addition to cyclopropane ring. Hydrogenation of double/triple bonds and aromatic rings. Hydroboration, Ene-reaction, Michael reaction and Sharpless assymetric epoxidation.

Unit-III Molecular Rearrangements (16 Contact hours)

General mechanistic treatment of nucleophilic, electrophilic and free radical rearrangments. Nature of migration and migratory aptitude and memory effect. Detailed study of following rearrangements: Wagner-Meerwein, Pinacol- Pinacolone, Demyanov, Benzil-Benzilic acid, Favorskii, Arndt-Eistert, Neber, Hofmann, Curtius, Lossen, Schmidt, Beckmann, Baeyer-Villiger, Pyne and Dienone - phenol rearrangements.

Unit-IV Pericyclic reactions. (16 Contact hours)

Molecular orbital symmetry, Frontier orbitals of ethene, 1,3- butadiene, 1,3,5-hexatriene and allylic systems. HOMO, LUMO concept, FMO approach. Classification of Pericyclic reactions. Woodward Hofmann rules for the following pericyclic reactions. Cycloadditions: Thermal and Photochemical 2+2 and 4+2 cycloadditions. Suprafacial and antrafacial cycloadditions.

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

Sigmatropic rearrangements: Classification, [1,3], [1,5] and [3,3] sigmatropic shifts. Cope and Claisen rearrangements. Suprafacial and antrafacial shifts of hydrogen atom.

Books Recommended

1. Advanced Organic Chemistry Reactions, Mechanism and Structure, 4th Ed.,Jerry March. (Wiley, 1999).
2. Advanced Organic Chemistry 4th Ed. - F. A. Carey and R. J. Sundberg. (Plenum, 2001).
3. A Guide Book to Mechanism in Organic Chemistry 6th Ed.- Peter Sykes. (Longman, 1996).
4. Structure and Mechanism in Organic Chemistry 2nd Ed. - C. K. Ingold. (CBS, 1994).
5. Modern Organic Reactions 2nd Ed. - H.O. House (Benjamin, 1972)
6. Principles of Organic Synthesis 2nd Ed. - R.O.C. Norman (Chapmann Hall, 1978)
7. Reaction Mechanism in Organic Chemistry 3rd Ed. - S.M. Mykherjee and S.P. Singh. Macmillan, 1998).
8. Organic Chemistry - J. Hornback,pk. (Brooks/Cole, 1998).
9. Fundamentals of Organic Cbemjstry , 5th ed.- Solomons. (Wiley, 1992).
10. Organic Chemistry, 5th Ed.- John McMurry. (Brooks/Cole, 2000).

Course No: CH17203CR

Title: Physical Chemistry (04 Credits)

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

Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*

End Term Exam (units III & IV): *50 Marks*

Unit-I 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.

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.

Ion solvent Interactions*:* Non structural (Born) treatment and an introduction to structural (Ion-dipole, Ion-quadruple) 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.

Unit-III Biophysical Chemistry (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 (synthesis & hydrolysis), Principles of coupled reactions and their importance for living systems.

Biopolymers: Molecular forces and Chemical bonding in Bio-polymers, hydrophobic interactions, structure of proteins, protein folding and unfolding. Biological membranes, phase transitions in biological membranes. Donan effect and transport across biological membranes.

Binding of Ligands and metal Ions to bio-macromolecules, one binding site per macromolecule, n equivalent binding sites per macromolecule, binding of oxygen to myoglobin and hemoglobin.

Unit-IV Statistical Thermodynamics (16 Contact hours)

Concept of distribution, thermodynamic probability and most probable distribution. Sterling approximation. Method of undetermined multipliers.

Distribution Laws: Derivation of Boltzmann distribution law, Bose-Einstein and Fermi-Dirac laws (without derivation) and their comparison with Boltzmann distribution law.

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

Books Recommended:

1. Physical Chemistry –P. W. Atkins, 9th Edition, 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, Lioyd L Lee, World Scientific, 2008.
7. An Introduction to Aqueous Electrolyte Solutions, Margaret Robson Wright, Wiley, 2007.
8. Modern Electrochemistry 1, 2A, 2nd Edition, J. O`M. Bokris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.
9. Physical Chemistry for the Biosciences, Raymond Chang, University Science Books, 2005.
10. Physical Chemistry for the Life Sciences,2nd Edition, Peter Atkins, Julio de Paula, Oxford University Press2015.
11. Statistical Thermodynamics, M.C.Gupta, New Age International, 1993.
12. Statistical Mechanics, Agarwal, Eisner, Wiley, 1991.

Course No: CH17204DCE

Title: Laboratory Course in Organic Chemistry (04 Credits)

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

External Exam: *80 Marks.* ***Internal Assessment****: 20 Marks*

1. **Qualitative Analyses of Organic Compounds**
   (i) **Physical Properties:** Physical state, colour, odour, solubility behavior 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, Nitrocompounds and Hydrocarbons.
   (iii) **Preparation and recrystallization of the derivatives of above mentioned group of compounds.**
2. **Separation, Purification and identification of Organic compounds from a three component mixture:**
   (a) **Separation based on solubility in water and organic solvents.**
   (b) **Separation based on Chemical properties:** Solubility in Sodium bicarbonate, Sodium Hydroxide and Hydrochloric acid.
   (c) **Identification of individual components using physico-chemical properties**
3. **Detection of functional groups using IR spectroscopy (spectra to be provided)**
4. **Quantitative Estimation of the following compounds**
   (a) Glucose.
   (b) Glycine
   (c) Acetone
   (d) Phenol.
   (e) Ascorbic acid.

5. Organic Preparations

(a) Acetylation of Cholesterol or salicylic acid.

(b) Oxidation of Cyclohexanol by chromic acid to get adipic acid.

(c) Aldol condensation: Dibenzal acetone and benzaldehyde.

(d) Cannizarro's reaction of 4-Chlorobenzaldelyde.

(e) Aromatic electrophillic substitutions in benzene, benzoic acid or aniline.

(f) Beckman rearrangement starting from acetophenone.

(g) Haloform reaction: Preparation of Iodoform.

Books Recommended:

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

Course No: CH17205DCE
Title: NMR and ESR Spectroscopy (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I NMR Spectroscopy-I (08 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 (T1, T2). Shielding and deshielding of magnetic nuclei. Chemical shift, its measurement and factors influencing chemical shifts; local paramagnetic and diamagnetic shielding, neighboring group anisotropy and ring currents in aromatic systems

Unit-II NMR Spectroscopy-II (08 Contact hours)

Spin- Spin coupling, coupling constants. Examples.

Vicinal coupling and electron correlation. Chemical equivalence and magnetic equivalence.

Fermi contact and Dirac Vector Model. Effect of Chemical exchange on spectra.

Double resonance techniques; spin decoupling, nuclear overhauser enhancement.

Instrumentation; FT-NMR and its advantages. NMR studies of nuclei other than proton – ^{13}C, ^{19}F and ^{31}P.

Unit-III ESR spectroscopy-I (08 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

Unit-IV ESR spectroscopy-II (08 Contact hours)

Fermi contact, Spin polarization effects, Dipolar coupling, Mc Conell equation and calculation of spin densities in inorganic radicals such as $CO_2^{-\bullet}$, $CH_3^{\bullet}$, $BH_3^{-\bullet}$ and $F_2^{-\bullet}$.

Spin orbit coupling and significance of g tensors.

Zero field splitting and Kramer's degeneracy (fine structure),

Advance Applications

Books Recommended

1. Introduction to Spectroscopy; 3rd edn.; D. L. Pavia, G. M. Lampman, G. S. Kriz; Saunders-Thomson learning; 2001.
2. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry; R. V. Parish; Ellis Horwood; 1990.
3. Nuclear Magnetic Resonance; P. J. Hore; Oxford; 1995.
4. Principles of Instrumental Analysis; 4th edn.; D. A. Skoog, J. J. Leary; Saunders; 1992.
5. Physical Methods for Chemists; 2nd edn.; R. S. Drago; Saunders; 1992.
6. Basic Principles of Spectroscopy; R. Chang; McGraw Hill; 1971.
7. Introduction to Magnetic Resonance; A Carrington, A. D. McLachlan; Harper & Row; 1967.
8. NMR and Chemistry; 2nd edn.; J. W. Akitt; Chapman and Hall; 1983.

Course No: CH17206DCE
Title: Solid State Chemistry (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Structure and Theories of Solids (16 Contact hours)

Structure of solids: 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. *S*tructure 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, Colour centres, Dislocations and their types.

Theories of solids:

Free electron theory of metals**:** The Drude Model, Lorentz modification, Sommerfield Model; Fermi-Dirac distribution function, Density of states, electronic heat capacity, Hall effect.

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. 10^{th}, 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: CH17207GE
Title: Metal Ions in Living Systems (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Alkali and Alkaline Earth Metal-ions in Biosystems (16 Contact hours)

Biomolecules and their Metal Coordination behavior.

Evidence of the presence of metal ions in biological systems (Direct / Indirect). Classification of metals and non-metals according to their action in biological systems.

Essential Elements: Concept of essentiality, criteria and classification of essential elements as per their role in living systems.

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.

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. Dioxygen transport (Haemocyanin).

Zinc in Biosystems: Lewis acid catalyst, Enzyme activator in vitamin B_{12}.

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

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

Antibacterial, Antiviral and Antifungal activities of metal complexes: Labile and Robust metal complexes; probable mechanism of action.

Books Recommended

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

Course No: CH17208GE
Title: Bio-Physical Chemistry (02 Credits)

Max. Marks: *50* — ***Duration:*** *32 Contact hours*

Ist Unit Exam: *25 marks* — ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Bioenergetics & Equilibrium in biological Systems (16 Contact hours)

Relevence of thermodynamics to Biological systems, Biochemists standard state, standard energy changes in biochemical reactions, ATP as energy currency of cell (synthesis & hydrolysis). Principles of coupled reactions and their importance for living systems.

Acid–base Equilibria: pH, pKa & pKb values. Dissociation of Amino-acids, isoelectric point. Buffer solutions, buffer capacity, effect of ionic strength & temperature, maintaining pH of blood.

Electrochemical equilibria: Standard redox potential, half- cell potentials of biological reactions, Nernst Equation.

Biological Membranes, Transport of ions across biological membranes, active and passive transport. Theory of membrane potential.

Unit-II Bio-electrochemistry, Kinetics & Spectroscopy (16 Contact hours)

Electrochemistry of Nerve conduction, medical applications of electrochemistry.

Renaturation of DNA as a second order reaction, Enzyme kinetics, Michaelis-Menton mechanism, competition & inhibition, multisubstrate systems, effect of substrate concentration, temperature and pH.

Fluorescence spectroscopy: Simple theory, excited state properties, florescence quenching, molecular rulers (FRET), single molecule florescence, applications in biological systems.

ORD and CD spectroscopy: Polarization of light and optical rotation, Optical rotatory dispersion and Circular dichroism, Circular dichroism of nucleic acids and proteins.

Books Recommended:

1. Physical Chemistry for life sciences; 2nd edn.; P. W. Atkins and J.D. Paula; Oxford University Press; 2010.
2. Fundamentals of general Biological Chemistry; 4th edn.; John . R. Holum; Wiley; 1990.
3. Principles of biochemistry; 3rd edn.; David. L .Nelson, Michael .M.Cox; Worth Pub.; 2002.
4. Physical Chemistry, Principles and applications in biological systems. 4thedn. Tinoco, Sauer, Wang, Puglisi. Pearson education, 2007.
5. Biophysical Chemistry; 2ndedn.; Alan Cooper; RSC. Publishing; 2011.

Course No: CH17209OE
Title: Chemistry of Bio-molecules (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

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

Oils and Fats: Fatty acids and Triglycerides. Saturated and Unsaturated fatty acids (MUFA and PUFA). Rancidity of Oils & Fats. Absorption of toxic substances by fat.
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.
Minerals: Macro and Micro minerals. Their functions and diseases caused by their deficiencies.

Books Recommended

1. Organic Chemistry; 5^{th} edn;. Vol.2,1.L. Finar (Addison Wesley Longman-2000).
2. Biochemistry, Biotechnology and Clinical Chemistry of Enzymes; Trevor Palmer (EWP). Organic Chemistry by I.L.Finar; Vol. II (ELBS Longamnn).
3. Lehninger's Principles of Bio-chemistry; D.L. Nelson; M.Cox Worth publications; 2000.
4. Introduction to Nucleic Acids and Related Natural Products; Ulbight; Oldborn Press.
5. Chemsitry of Natural Products; S.V. Bhat, B.A. Nagasampagi, M. Siva Kumar. Naroosa Publishing House; New Delhi.

Course No: CH17301CR
Title: Selected Topics in Inorganic Chemistry (04 Credits)

***Max. Marks:** 100* — ***Duration:** 64 Contact hours*
***Ist Unit Exam:** 25 marks* — ***IInd Unit Exam:** 25 marks*
***End Term Exam (Units III & IV):** 50 Marks*

Unit-I Metal-ions in Biological Systems: (16 Contact hours)

The role of metal-ions in Metal-Protein systems; in trigger and control mechanisms; in structural context; as Lewis acid and as redox catalysts.

Biodistribution and biochemical role of essential trace and ultra-trace elements:- Fe, Zn, Cu, V, Cr, Mn, Ni, P, F and I. Effects of their deficiencies and treatment.

Antagonism and Synergism among essential trace elements.

Alkali and Alkaline earth metal ions (Na^+, K^+, Ca^{2+} & Mg^{2+}): Biological role; ligands and mechanism of ion transport (Facilitated transport, Carriers, Channeling and active transport of Cations).

Role of Lithium in mental health.

Chlorophyll: Structure and role of magnesium in photosynthesis.

Biological Nitrogen Fixation: Dinitrogen Complexes and their reactivity; Nitrogenase enzyme; Fixation via nitride formation.

Unit-II Bonding in Main Group Compounds (16 Contact hours)

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 Compounds (Borazine), Phosphorous–Nitrogen compounds (Cyclophosphazenes, polyphosphazenes and phosphonitrillic halides), Sulphur-Nitrogen compounds (polythiazyls and Sulphur Nitrides)

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 μ_s and μ_{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.

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.

Unit-IV NQR & Mossbauer Spectroscopy. (16 Contact hours)

Basic principles, Spectral parameters such as isomer shift, quadrupole splitting and magnetic splitting, spectrum display.

Application of the technique to the studies of (i) bonding and structure of Fe^{2+} and Fe^{3+} compounds including those of intermediate spin, (ii) Sn^{2+} and Sn^{4+} compounds— nature of M—L bond, coordination number and structure, (iii) detection of oxidation state and inequivalent MB atoms.

NQR isotopes, Nuclear quadruple moment; Electric field gradient; nuclear quadruple coupling constant; Effect of applied magnetic field, Applications.

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; IInd 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. Infrared and Raman Spectra: Inorganic and Coordination compounds ; K. Nakamoto; Wiley.
11. NMR, NQR and Mossbauer Spectrascopy in Inorganic Chemistry ; R.V.Parish; Ellis Horwood.

Course No: CH17302CR
Title: Organic Chemistry (Spectroscopy & Photochemistry) (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (Units III & IV): *50 Marks*

Unit-I Applications of Spectroscopy: (16 Contact hours)

Recapitulation of UV, IR Spectroscopy, Woodward-Fieser rule Characteristic absorptions of various functional groups. Interpretation of IR Spectra.

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. Mass Analyzer Determination of Molecular Formula, Role of Isotopes, Nitrogen Rule, Metastable Peak. Fragmentation pattern like Stevenson rule , initial ionization event, α-cleavage, inductive cleavage, two bond cleavage, Retro-Diels. Alder cleavage, McLaffertey Rearrangements. Fragmentation pattern of alkanes, alkenes, alcohols, phenols, aldehydes, ketones, Carboxylic acids, Amines, Problems based on Mass Spectroscopy. Some specific examples from natural products like flavanoids terpenes, steroids, alkaloids.

Unit-II Nuclear Magnetic Resonance 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 A_2, AB, AX, AB_2, AX_2, A_2B_2. Proton exchange, deuterium exchange, Peak broadening exchange

C-13 NMR : Carbon 13-chemical shifts , proton coupled and decoupled spectra. Nuclear overhouser, Effect, Off-Resonance De-coupling, A quick dip in to DEPT-45 , DEPT-90, DEPT-135.

Introduction to two-dimensional spectroscopy methods, Cosy techniques, HETCOR technique, OESY, combined structure problems.

Unit-III Photochemistry-I. (16 Contact hours)

Photochemical Reactions

Interaction of electromagnetic radiation with matter. Types of excitations. Singlet and triplet states and their lifetimes. Fate of excited molecule: Physical and chemical processes. Transfer of excitation energy: Sensitization and Quenching. Quantum yield. Types of photochemical reactions.

Photochemistry of alkenes

Geometrical isomerisations, cyclisation and dimerisation reactions. Photochemical reactions of 1,3- butadiene (excluding pericyclic reactions). Rearrangements of 1,4 and 1,5- dienes.

Photochemistry of saturated carbonyl compounds

Intramolecular reactions of saturated acyclic and cyclic carbonyl compounds. (Norrish type-I and Norrish type-II processess). Intermolecular cycloaddition reactions (Paterno- Buchi reaction).

Unit-IV Photochemistry –II. (16 Contact hours)

Photochemistry of unsaturated carbonyl compounds

Photochemical reactions of α, β-unsaturated carbonyl compounds. (H-Abstraction and isomerisation to β, γ-unsaturated carbonyl compounds). Photolysis of cyclic α, β-unsaturated ketones (dimerisation and lumiketone rearrangement) and cyclohexadienones.

Photochemistry of Aromatic compounds

Photoinduced isomerisations of benzene and its alkyl derivatives. 1,2 ; 1,3 and 1,4 photoaddition reactions of benzene. Nueleophilic photosubstitution reactions in aromatic compounds. Photo Fries-rearrangement of aryl esters and anilides.

Miscellaneous Photochemical reaction

Photolysis of organic nitrites and their synthetic utility (Barton reaction).

Photochemistry of vision.

Books recommened:

1. Spectrometric identification of Organic Compounds. 5th Ed., R.M.Silverstein, G.C.Bassler and T.C.Morill. (Jhon 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. Intoductory Photochemistry, A.Cox and T.Kemp (McGraw Hall-1971).
6. Organic Photochemistry, 2nd Ed., J.Coxon, and B.Halton (2nd Ed. Cambridge University press-1987).
7. Fundamentals of photochemistry, Rohtagi & Mukherjee (Wiley Eastern-1992).

Course No: CH17303CR
Title: Physical Chemistry (04 Credits)

Max. Marks: *100* | ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit Exam:*** *25 marks*
End Term Exam (Units III & IV): *50 Marks*

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 pi-bond-order. Alternant hydrocarbons, Naphthalene. 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-Fockself consistent field method. One and two-electron integrals in the light of minimal basis H_2 system

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 Electrochemistry-I (16 Contact hours)

Conductance of electrolyte solutions: Mobility of ions, mobility and conductivity, Einstein relations, dependence of molar conductance on concentration, estimation of K and Λ^0 for weak electrolytes, Theories of Conductance: Debye-Huckel-Onsager conductance equation and brief idea of its extension.

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, recent advances.

Semiconductor electrodes: Structure of seminconductor/electrolyte interface.

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

Theories of Heterogeneous Electron Transfer: Electron transfer at electrified interface at and away from equilibrium. Butller-Volmer equation, low and high field approximations, significance of transfer coefficient.

Electrochemistry in Materials Science: Corrosion, types and mechanism of corrosion, corrosion current, corrosion potential, Electrodics of corrosion in absence of Oxide films; Monitoring and inhibition of corrosion; cathodic and anodic protection, passivation.

Photoelectrochemistry: Band bending across Semiconductor/electrolyte solution interface, photoelectrochemistry across semiconductor/electrolyte interfaces, p-type photocathode, n-type-photoanode, surface effects in photoelectrochemitry, photoelectrochemical splitting of water, photoelectrochemical reduction of CO_2.

Books Recommended:

1. Physical Chemistry –P. W. Atkins, 9th Edition, 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, Tata McGraw 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. M. J. Rosen, J. T. Kunjappu, “Surfactants and Interfacial Phenomena”, John Wiley & Sons, New York, 4th Edition, 2012.
7. D. Y. Meyer, “Surfaces, Interfaces and Colloid”, VCH Publishers, Inc. 1991.
8. Jonsson, Lindmann, Homberg and Kronberg, “Surfactants and polymers in aqueous solution”, John Wiley and sons, 1998.
9. Molecular Thermodynamics of Electrolyte Solutions, Lioyd L Lee, World Scientific, 2008.
10. An Introduction to Aqueous Electrolyte Solutions, Margaret Robson Wright, Wiley, 2007.
11. Modern Electrochemistry 1, 2A,2B 2nd Edition, J. O`M. Bokris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.
12. Electrochemical methods, Fundamentals and Methods, A.J. Bard, L.R. Faulkner, Wiley, 1980.
13. Physical Electrochemistry- Fundamentals, Techniques and Applications, Eliezer Gileadi, Wiley-VCH 2011.
14. Electrochemistry, 2nd Edition, Carl H. Hamann, Andrew Hammett, Wolf Vielstich, Wiley-VCH.

Course No: CH17304DCE

Title: Laboratory Course in Physical Chemistry (04 Credits)

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

***External Exam:** 80 Marks.* | ***Internal Assessment**: 20 Marks*

A. Conductometry

1. Determination of the composition of a mixture of HCl and CH_3COOH by titration with standard NaOH.
2. Determination of degree of dissociation of a weak acid.

B. Potentiometry

1. Determination of strength and pKa value of weak acid by titration with an alkali using quinhydrone electrode.
2. Titration of Fe (II) vs. $K_2Cr_2O_7$ and determination of standard redox potential of Fe^{2+}/Fe^{3+}.

C. pH-metry

1. Determination of pKa values of a tribasic acid by titration with an alkali.
2. Determination of degree of hydrolysis of aniline hydrochloride.

D. 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.

E. Spectrophotometry

1. Determination of composition of a binary mixture of $K_2Cr_2O_7$ and $KMnO_4$ or Cobalt (II) and Nickel (II) ions.
2. Spectrophotometric titration of Fe(II) vs. $KMNO_4$.

F. 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.

G. Viscometry

1. Investigation of variation of viscosity with conc. and determination of unknown concentration.
2. Determination of the radius of a molecule by viscosity measurement.

Books Recommended:

1. Practical Physical Chemistry, Findley, Kitchener, Longman, 1977.
2. Advanced Practical Physical Chemistry, Yadav , Goel Pub, 1994.
3. Experiments in Physical Chemistry, 5th ed., Schoemaker et al. , MGH, 1989.

Course No: CH17305DCE
Title: Chromatographic Techniques (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

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; 5th Edition; F. W. Fifield, D. Kealey; Blackwell Sciences Ltd.; 2000.
2. Modern Analytical Chemistry; David Harvey; McGraw-Hill; 2000.
3. Chromatographic Methods; 5th edn. ; A. Braithwaite and F. J. Smith; Kluwer Academic Publishers.
4. Fundamentals of Analytical Chemistry; 6th 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: CH17306DCE
Title: Non-Equilibrium Thermodynamics (02 Credits)

***Max. Marks:** 50* | ***Duration:** 32 Contact hours*
***Ist Unit Exam:** 25 marks* | ***IInd Unit (Term end) Exam:** 25 marks*

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 stationery 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 IrreversibleProcesses;DeGroot,Mazur;Dover;1986.
2. Introduction to Thermodynamics of Irreversible Processes; I.Prigogine; Wiley Interscience; 1967.
3. Thermodynamics for students of Chemsitry, Kuriacose, Rajaram, (S. ChandandCo., 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-equlibrium thermodynamics, 2nd ed. Yasar Demirel. Elsevier, 2007.

Course No: CH17307GE
Title: Industrial Pollution and Green Chemistry (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Industrial Pollution and Environmental Toxicology (16 Contact hours)

Industrial Pollution: Cement, Sugar, Drug, Paper and pulp. Thermal power plants, Nuclear power plants and Polymers.

Radio nuclide analysis: Disposal of wastes and their management.

Principles of Toxicology, Dose Response Relationship, risk assessment and management.

Organochlorine Compounds: Accumulation and fate in biological systems. Toxicology of PCBs. Dioxins and Furans, Health effects in humans.

Environmental Estrogens.

Unit-II Green Chemistry (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 and Sonication.

Green Solvents and Reaction conditions: Supracritical fluids, aqueous reaction conditions, immobilized Solvents and irradiative reaction conditions.

Examples of Green materials, reagents and some specific reactions.

Books Recommended

1. Environmental Chemistry; 8th edn.; S. E. Manahan; CRC Press; 2005.
2. Chemistry of the Environment; IInd edn.; T. G. Spiro and W. M. Stigliani; Prentice Hall; 2002.
3. Environmental Chemistry; IInd edn.; Colin Baird; Freeman & Co.; 1991.
4. Chemistry of the Environment; IInd Edn. R. A. Bailey; H. M. Clark; J. P. Ferris; S. Krause & R. L. Strong; Elsevier; 2005.
5. Environmental Chemistry; IInd edn.; Samir K. Banergi; Prentice- Hall; 2001.
6. Green Chemistry- Environment Friendly Alternatives; Rashmi Sangh & M. M Srivastava; Narosa; 2007.
7. Green Chemistry- An Introductory Text; IInd Edn.; Mike Lancaster; RSC; 2010.
8. Green Chemistry- Theory and Practice; P. T. Anastas and J. C. Warner; oxford; 2000.
9. Green Chemistry; Ist Edn.; Samuel Delvin; IVY Publishing House; 2008.
10. Green Chemistry- Environmentally Benign Reactions; V. K. Ahluwalia; Ane Books; 2006.

Course No: CH17308GE
Title: Bio-Organic Chemistry (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I (16 Contact hours)

(a) Chemical Origins of Biology

Bio organic chemistry: Introduction ,Basic consideration , Proximity effects in Organic Chemistry , Molecular rearrangments.

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 Nomeclature 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+ and NADP+), Flavin Nucleotides (FMN and FAD), Adenosine phosphate (ATP, ADP, AMP) .

Coenzyme A (CoA -SH) ,Thiamine Phosphate, Biotin, Tetrahydrofolate, Coenzyme B_{12} .

(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 Gregary Weiss; Taylor and francis. 2013.
2. Bio-organicchemistry : Harman Dugas 3rd ed.Springer (2010) .
3. Bio-organic chemistry J.Rohr ,Springer (2000).
4. Enzymes 2nd ed. T. Palmer and P. Bonner (2008).
5. Biochemistry :Donald Voet, Judith.G. Voet 2nd ed.Willey (1995)

Course No: CH17309OE
Title: Philosophy of Science (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Representation (08 contact hours)

Laws of nature**:** Knowledge**, S**ources of knowledge, The rationalists, The empiricists, The Mathematical knowledge, Synthetic Knowledge, Science as knowledge source, Religion and science The Method of science, Induction versus deduction, Representation and reason, Probabilistic laws, Basic and derived laws,

Realism: Realism and its critics, Instrumentalism, Constructive empiricism, Laws and antirealism, Anti-realism and structure of science.

Unit-II Reason (08 contact hours)

Inductive Scepticism: Theory and observation, Dissolving the problem of Induction, Probability
and scientific inference, Kinds of Probability,

Inductive Knowledge: Reliabilist epistemology, reasoning with induction, Innate epistemic capacities and reasoning about induction, Internalism and justification.

Method and Progress: Methodology of scientific research programmes, Clinical trials and the scientific method, The content of discovery and the context of justification, Science without the scientific method, Method and the development of sciences, Paradigms and Progress.

Unit-III Classical Determinism and Probabilistic world (08 contact hours)

The Classical Mechanics: Mechanistic determinism, General principles; Action at a distance, Electric and magnetic forces, Failures of the classical mechanics;
Atomic structure, problem of radiation.

The birth of modern science**:** The photo-electric effect**,** The atomicity of radiation, Particle wave duality, waves of probability, Uncertainty principle, subject versus object, the fundamental laws of radioactivity, The new Quantum theory, wave mechanics, Diracs Quantum mechanics, The new philosophical principles, the probabilistic reasoning.

Unit-IV The Dawn of Modern Thinking (08 contact hours)

The arrow of Time: From Descarts to quantum theory, the relation of quantum theory to other natural sciences. Language and reality in modern science. The role of modern science in the present development of human thinking.

Books Recommended:

1. Philosophy of science; Alexander Bird; McGill-Queen's University Press.
2. Physics and Philosophy; W. Heisenberg; Harper Perennial Modern Classics.
3. Physics and Philosophy; Sir James Jeans; Cambridge University Press.
4. Reconstruction of religious thought in Islam; Muhammad Iqbal; Adam Publishers & Dodo Press.
5. Philosophy of natural science; Carl G. Hempel**;** Pearson.
6. The philosophy of science; David Papineaus; Oxford University Press.
7. Reality and Representation; David Papineaus; Blackwell Publication.
8. Belief, truth and knowledge; D.M. Armstrong; Cambridge University Press.
9. Modern epistemology; Nicholas Everitt and Alec Fisher; McGraw-Hill Higher Education.
10. The structure of scientific revolution; Thomas S. Kuhn; The University of Chicago Press

Course No: CH17401CR
Title: Organo-Transition Metal Chemistry (04 Credits)

Max. Marks: *100* — ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Sigma Bonded Organometallic Compounds: (16 Contact hours)

Classification, Stability, Comparison to main Organometallic Compounds, Routes of synthesis, Reactions. Decomposition Pathways: Choice, α and β hydrogen transfer. Intramolecular elimination of alkane, Cyclometallation, Stability from bulky substituents, Agostic alkyls, Umpolung.Metal Hydride Complexes: Synthesis, Characterization and Chemical reactions, Non-classical Hydrides (Kubas complexes).

Unit-II Pi-bonded Organometallic Compounds: (16 Contact hours)

Classification, Structure and bonding in Metal- alkene, alkyne, allyl, 1,3-butadiene and Cyclobutadiene Complexes.

Sandwich Compounds: Characteristics; Classification, Synthesis, Reactions, 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.

Unit-III Catalytic Processes involving Transition Metal Organometallic Compounds: (16 Contact hours)

Mechanistic aspects: Oxidative addition, Insertion reactions Reductive elimination and water gas shift reaction (WGSR).

Catalytic mechanism of Hydrogenation, Hydroformylation, Oxidation and Isomerization of alkenes; Olefin metathesis.

Fischer-Tropsch Synthesis and Ziegler Natta polymerization of alkenes.

Asymmeteric and supported Organometallic Catalysis (brief idea)

Unit-IV Fluxional Organometallic Compounds and Synthetic Reactions involving Organo- metallics (16 Contact hours)

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 η^1 Cyclopentadienyls and η^3–allyls.

Stereochemical non rigidity in case of coordination numbers- 4 & 5 (cis-trans, atomic inversion, Berry Pseudorotation).

Synthetic Reactions involving Organo- metallics:

Reactions of coordinated ligands, carbon monoxide, alkyls, alkenes (Green, Mingo's rules).

Activation of small molecules: Carbon monoxide, Carbon dioxide and Alkanes.

Role of organo-iron as synthons, Carbon-Carbon coupling and its reactions (Suzuki and Heck).

Books Recommended:

1. The Organometallic Chemistry of Transition Metals; 2nd edn; Robert. H . Crabtree; Wiley; 1994.
2. Fundamental Transition Metal Organometallic Chemistry; Luke hart; Brooks / Cole; 1985.
3. Organometallic Chemistry; 2nd edn ; Mehrotra & Singh ; New age international 2000
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 press 1983.
9. Reaction Mechanism of Inorganic and Organometallic systems; 2nd edn.; Robert .b. Jordan 1998.
10. Inorganic Chemistry ; 4th edn.; Huheey ; E. Keiter & R. Keiter; Addison-Wesley ;1983
11. Modern Inorganic Chemistry; William. A. Jolly; McGraw Hill; 1985.

Course No: CH17402CR
Title: Photo-Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Basics of Photo-Chemistry (16 Contact hours)

Absorption; mechanism of absorption of light

Transition moment integral, Einstein's treatment, molar integrated absorption intensity, natural radiative lifetime & the calculation of life times.

Excitation; d-d transition, charge transfer & intraligand 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 diagramsdepicting excited states.

Frank Condon principle, shapes of absorption & emission bands.

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

Tools and Technique: Light source, measurement of light intensity, chemical actinometry. Flash photolysis.

Unit-II The Chemistry of Excited State Molecules (16 Contact hours)

Photochemical laws & quantum yield. Kinetics & quantum yield of photo-physical (radiative) and photo-chemical processes. Photochemical processes: primary, secondary, adiabatic & non- adiabatic. Properties of thexi states; Determination of dipole moments & acidity constants of excited state molecules.

Photosubstitution and photo reduction of Co (III) complexes.Photosubstitution reaction of Cr (III) and Rh (III) complexes.

Organometallic-Photochemistry: Reactions of metal carbonyls, cleavage of metal-metal bond.

Unit-III Redox Reactions by Excited Metal Complexes (16 Contact hours)

Energy transfer under conditions of weak and strong interaction. Excited state electron transfer. Marcus-Hush model.Conditions of the excited states to be useful as redox reactants. Photochemical electron transfer, [Ru (bipy)3]2+ and [Os (bipy)3]2+.

Photochemical supramolecular devices: devices for photo-induced energy or electron transfer, Devices for information processing, photo-chemically driven molecular machines.

Unit-IV Solar Energy-Prospects and Challenges (16 Contact hours)

Solar energy storage, solar energy conversion, Metal complex sensitizers and electron relays in photochemical splitting of water, Nitrogen fixation and CO_2 reduction. Inorganic photolithography.

Supramolecular photochemistry in natural systems: photosynthesis, bacterial photosynthesis and artificial photosynthesis.

Books Recommended:

1. Reaction Mechanisms of Inorganic and Organometallic Systems; 2nd edn.; Jordon; Oxford; 1998.
2. Mechanism of Inorganic Reactions; Katakis, Gordon; Wiley; 1987.
3. Inorganic Chemistry; 4* edn; Huheey; Harper & Row; 1990.
4. Mechanism of Inorganic Reactions, 2nd edn, Basalo, Pearson; Wiley Eastern, 1997.
5. Chemistry of Light; Suppan, Royal Society; 1994.
6. Photochemistry, Carol J. Wayne and Richard P. Wayne; Oxford University Press; 1996.
7. Fundamentals of Photochemistry; C Rohatgi, Mukhergi; Wiley Eastern.; 1992
8. Inorganic Photochemistry; J.Chem Edu.;Vol .60, No.10,1983.
9. Applications of Inorganic Photochemistry; J. Chem. Edu.; Vol.74, No 69. 1997.

Course No: CH17403CR
Title: Bio-Inorganic Chemistry (04 Credits)

Max. Marks: *100* — ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Iron Storage, Transport and Oxygen carriers: (16 Contact hours)

Structure and Coordinating sites in biologically important ligands: Proteins, Nucleotides and Lipids.

The transport mechanism: uniport, symport and antiport.

Ferritin and Transferrin: Structure, Metal binding sites; incorporation and release of iron.

Porphyrins: Introduction, characteristic absorption spectrum and salient characteristics.

Haemoglobin and Myoglobin: Structure, oxygen saturation curves; Mechanism of oxygen transport and storage.Bohr effect and cooperativity in haemoglobin.

Hemerythrin and Hemocyanin: Structure, Metal binding groups and Dioxygen binding. Synthetic oxygen carrier model compounds: Vaska's iridium complex: Cobalt complexes with micro and macrocyclic ligands and Schiff base ligands.

Unit-II Metallo-enzymes and Electron Carriers (16 Contact hours)

Enzyme, Apoenzyme, Coenzyme, Prosthetic group and Metalloenzymes, Mechanism of enzyme action.

Zinc enzymes:- Carboxypeptadiase and Carbonic Anhydrase : Introduction, Structure, Mechanism of action and their model compounds.

Biological chemistry of Molybednum: uptake of Molybednum; oxidation states and redox potentials in enzymes and oxygen atom transfer reactions.

Xanthine oxidase and Aldehyde oxidase: Structure and biological role.

Cobalt in Vitamin B_{12}: Introduction, Structure and Derivatives of B_{12} and mechanism of alkylation reaction. Role of vitamin B_{12}.

Electron Carriers: Rubredoxin & Ferridoxin (Structure and biological role).

Blue Copper proteins: Oxidases and Plastocyanin (Structure and biological role).

Unit-III Metal-ion Induced Toxicity and Chelation Therapy (16 Contact hours)

Toxic levels of different metals. Sources of metal ion poisoning (external sources and internal disorders).

Mechanism of metal ion induced toxicity:- Toxicity of Pb, Cd, Hg, As, and CN- Metal ion promoted Carcinogenesis and probable mechanism of action.

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 Metal Salts and Metal Complexes in Therapeutics (16 Contact hours)

Treatment of essential metal deficiencies: Iron, Copper and Cobalt.Metal salts as anti-acids, antiseptic and diuretics.

Gold compounds and Rhematoid arthiritis.

Anti-Cancer Drugs: cis-Platin and its derivatives. Structure-function relationship.

Complexes of Rhodium, Gold and Cobalt.

Anti-bacterial, Anti-viral and Anti-fungal activities of Metal Complexes: Labile and Robust metal complexes; Probable mechanism of action.

Books Recommended:

1. As listed for Course No. CHM—101 (Inorganic chemistry-M.Sc. 1st Semester! From serial No. 1 to 5.
2. Bio inorganic Chemistry -An introduction; Ochai, Allyn and Bacon; 1977.
3. Inorganic Bio-chemistry—Vol. 1&2; Eichhorn; Elsevier, 1973.
4. Inorganic Aspects of Biological and Organic Chemistry; Hanzilik; Academic; 1976.
5. The Inorganic Chemistry of Biological processes; 2nd edn.; Hughes ; Wiley; 1973.
6. A Text book of Medicinal aspects of Bio inorganic Chemistry; Das; CBS; 1990.
7. The Biological Chemistry of Elements; Frausto de Silva; Williams; Clarenden; 1991.
8. Principles of Bio inorganic Chemistry; Lippard, Berg; Univ. Science Books; 1994.
9. Inorganic Chemistry in Biology; Wilkins C & Wilkins G; Oxford; 1997.
10. Bio inorganic Chemistry ; K. Hussain Reddy; New Age International (P) Ltd; 2005.
11. Metal -Ions in Biochemistry; P. K. Bhattacharya; Narosa Publishing House; 2005.

Course No: CH17404CR
Title: Heterocyclic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Structure and Nomenclature of Heterocyclic compounds (16 Contact hours)

Introduction and significance of heterocycles in day to day life.

Nomenclature of Heterocycles: Monocyclic, bicyclic and polycyclic heterocycles, Hantzsch-Widman and replacement methods of nomenclature.

Structural features: Non-aromatic, aromatic and heteroaeromatic heterocycles.

Tautomerism in heterocycles, Meso-ionic systems.

Spectroscopic properties of heterocycles (UV,Visible and ^{1}HNMR).

Unit-II General Approach to Synthesis of Heterocyclic compounds (16 Contact hours)

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 quinoline, Bischler-Napieralki Isoquinoline,Knorr Pyrrole,Paal-Knorr , Fischer – Indole synthesis.

Unit-III Monocyclic Heterocycles (16 Contact hours)

Structure, Synthesis and Reactions of Oxirane, Thirane, Azetidine, Pyrrole, Furan, Thiophene, Diazenes, Pyrimidines,Pyridine.Chemistry of five membered heterocycles with two heteroatoms like 1,3-Azoles, 1,2- Azoles. Chemistry of Six membered rings like Azines and seven membered heterocycles like Azepine,Oxipene,Thiepins.

Unit-IV Bicyclic Heterocycles (16 Contact hours)

Structure, Synthesis and reactions of Benzo- fused heterocycles like Benzo-pyrrole, Benzo-furan,Benzo-thiophene, Quinoline, Isoquinoline, Chromones, Coumarins, Iso-Coumarins, 2 and 4-benzopyrones, Benzopyryllium salts and purines.

Books Recommended:

1. Heterocyclic Chemistry, 5th Ed. J.A.Joule and K.Mills, (Wiley-2010).
2. Essentials of Organic Chemistry, Paul M Dewick , (Wiley-2006).
3. Heterocyclic Chemistry, J.A. Joule and G.F.Smith , (Chapman and Hall-1996).
4. The Chemistry of Heterocycles Theophil Eicher and Siegfried Hauptmann , (George Thieme Verlag Stutt gart,New York -1995).
5. Heterocyclic Chemistry, Raj K. Bansal, (New Age International Publisher-2006).
6. Heterocyclic Chemistry, R.R.Gupta,M.Kumar,V.Gupta,(Springer-2006).

Course No: CH17405CR
Title: Chemistry of Natural Products (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Terpenoids and Carotenoids (16 Contact hours)

Introduction, classification, general methods of isolation, separation.

Essential oils: Separation using Gas Liquid Chromatography and High Performance Liquid Chromatography. Physical, chemical and spectral methods of structure elucidation.

Structure determination, stereochemistry and synthesis of α-terpineol, abietic acid and β-carotene.

Unit-II Alkaloids (16 Contact hours)

Introduction, classification, nomenclature, qualitative tests, pharmaceutical applications and general methods of isolation. Physical, Chemical & Spectral methods of structure elucidation.

Stereochemistry, synthesis and biosynthesis of Quinine, Morphine and Reserpine.

Unit-III Steroids (16 Contact hours)

Introduction, nomenclature, classification & stereochemistry. Physical, Chemical & Spectral methods of characterization. Qualitative tests.

Cholesterol: Isolation, clinical significance, chemical properties, structure elucidation, total synthesis & relationship with bile acids.

Sex hormones: Introduction, isolation, clinical & commercial significance, color reactions, structure determination and partial synthesis of Oesterone, Androsterone, Testosterone and Progesterone.

Glucocorticoids & Mineral Corticoids: Introduction and partial synthesis of Cortisone, aldosterone and synthesis of cholecalciferol.

Unit-IV Natural Plant Pigments and Porphyrins (16 Contact hours)

Introduction, classification, physical, chemical, degradative and spectral methods of structure determination and biosynthesis (Acetate and Shikimic acid pathway)

Flavonoids: Isolation, separation and quantification. Antioxidant activity of flavonoids. Robinson's synthesis, Baker Venketraman synthesis, Kostanecki synthesis of flavanone and Flavanol.

Isolation, structure determination and synthesis of Cyanidin, Chrysin, Quercitin & Genestein.

Porphyrins: Structure determination and total synthesis of haemoglobin. Structural comparison with chlorophyll.

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. New Trends in Natural Product Chemistry, Atta-ur-Rahman (Harward Academic Press).
4. Chemistry of Natural Products, N.R. Krishnaswamy (University Press-1999).
5. Flavanoids; Oyvind M. Andersen and Kenneth R. Markhan. (Taylor & Francis -2006)

Course No: CH17406CR
Title: Bio-Organic and Medicinal Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I (16 Contact hours)

Vitamins:_ Source, structure and synthesis of vitamins – Vitamin A, Vitamin B-Complex (Thiamine riboflavin, folic acid); Vitamin B-12 (Structure only) Vitamin C, E, K, H and D.

Prostaglandins : Introduction and nomenclature, approaches to prostaglandin synthesis, cyclo-hexane, precursors-Woodward synthesis of PGF2a. Cyclo-heptane precursors - Corey's synthesis of prostoglandin's E & F.Their relationship with oxygenase I and II.

Nucleic Acids: Structure of nucleotide, nucleosides, RNA and DNA, role of nucleic acids in protein synthesis, genetic code and heredity. DNA finger printing

Unit-II (16 Contact hours)

Enzymes : Introduction, nomenclature & classification.. Activation & inhibhion of enzymes. Mechanism of enzyme action- Fischer lock and key, koshlands induced fit hypothesis, displacement reactions & coupling of ATP. Enzyme mechanism of chymotrypsin lysozyme & carboxypeptidase.

Co-Enzymes: Cofactors derived from vitamins, coenzymes, prosthetic groups. Apoenzyme. Structure , biological function and mechanism of reactions catalsed by co-enzymes: coenzyme A, thiamine pyrophosphate. pyridoxal phosphate, NAD+, NADP+, FMN, FAD and Lipoic acid.

Unit-III (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, carbonylic, thiols sulphides groups and introdction/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. Lipophillic constant, Hamett constant, steric parameters and Hansch analysis.

Unit-IV (16 Contact hours)

Antibiotics: Classifications-structural and mechanistic, cell wall biosynthesis inhibitors, protein synthesis inhibitors. Pencillins-classification and structures. Synthesis of Pencillins, V, G, chloroamphenicol.and ciprofloxacin. Tetracyclins.

Psychoactive Drugs: Introduction, CNS depressants, CNS stimulants, sedatives and hypnotics, barbutirates. Synthesis of diazepam, phenytoins and glutethisimide.

Anti-neoplastic drug: Introduction; cancer chemotherapy, carcenoolytic antibiotic, plant derived anti-cancer agents (Taxol)role of alkylative agents and antimetabolites in treatment of cancer, mitotic inhibitors (elementary idea).

Cardiovascular Drugs: Introduction, cardiovascular diseases, synthesis of Amylnitrate. sorbitrate, quinidine, verapanil, methyl dopa and atenolol

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, Biotechonolgy and Clinical Chemistry of Enzmyes. Trevor Palmer (EWP)
5. Organic Chemistry by I.L.Finar Vol. II (ELBS Longamnn)
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. Chemsitry of Natural Products. S.V. Bhat, B.A. Nagasampagi, M. Siva Kumar. Naroosa Publishing House, New Delhi.

Course No: CH17407CR
Title: Advanced Quantum Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Electronic Structure Theory, Hartree-Fock Method (16 Contact hours)

Review: Electronic Hamiltonian, antisymmetrized wave function, Slater determinant. Hartree-Fock self-consistent field method. One and two-electron integrals in the light of minimal basis H_2 system.

Hartree-Fock Equation, Fock, Coulomb and exchange operators and integrals, restricted Hartree-Fock formalism, Roothaan equation. The Fock matrix elements, Koopman's theorem, Slater-Condon rules. Matrix form of Roothaan equation, the SCF procedure.

Basis Sets: Slatter-type orbitals, Gaussian basis sets. Model SCF calculations on H_2 /$HeH^{+.}$

Unit-II Configuration Interaction and Semiempirical methods (16 Contact hours)

Configuration Interaction: Electron correlation, configuration state functions, configuration interaction (CI), Brillouin theorem, full and truncated CI theories- CID, CISD, CISDTQ methods; Size consistency problem. Moller-Plesset and Coupled Cluster methods.

Semiempirical methods: The ZDO approximation; the PPP method, brief idea of CNDO, INDO and NDDO methods. The MINDO, MNDO, AM1 and PM3 methods.

Unit-III Density Functional Methods and Molecular Properties (16 Contact hours)

Density Functional Theory:Electron probability density. Hohenberg-Kohn theorems, Kohn-Sham formulation of DFT, n- and v- representabilities, E_x&$E_c$functionals; the local density and local spin density approximations, gradient corrected and hybridfunctionals.
Brief idea of Molecular mechanics methods, force fields.

Molecular Properties*:* Potential energy surfaces; molecular geometry and its optimization, Hessian Matrix and normal modes, vibrational frequencies, thermodynamic properties. Dipole moments, atomic Charges.

Unit-IV Use of Quantum Chemistry Software: Gaussian (16 Contact hours)

A quick tour of GAUSSIAN Interface. Input to Gaussian. Model calculations illustrating various features of the package**..**

1. A single point energy calculation: HCHO /CH3.CHO,HCHOMOs.
2. Geometry Optimization: Input and Output for ethene, fluoroethene, propene conformers
3. Transition state optimization $CH_2O \rightarrow$ HCOH
4. NMR properties of ethane, ethene and ethyne.
5. Frequency Calculations: Input, Formaldehyde frequencies, Normal modes, zero point energy, thermodynamic properties, polarizability, hyperpolarazability.
6. Stationary points characterization –C3H5F
7. Model Chemistries: Basis set effect on HF bond length

8. Selecting an appropriate theoretical method:
   a) Electron correlation and post SCF methods, limitations of Hartree-Fock theory: HF bond energy, Optimization of O_3.
   b) Density Functional Theory: CO_2 structure and atomization energy.
   c) Butane / Isobutane isomerization energy, rotational barrier in n-butane.

9. Chemical reactions and reactivity:
   a) Hydration enthalpy of the reaction $H^+ + H_2O \rightarrow H_3O^+$
   b) Potential energy surfaces. Reaction path following (IRC calculation)
   $CH_2O \rightarrow HCOH$
   c) Heat of formation of CO_2 via an isodesmic reaction
10. Solvation models: Formaldehyde Frequencies in Acetonitrile

Books Recommended

1. Quantum Chemistry, Ira. N. Levine, (Prentice Hall, 2009).
2. Quantum Chemistry, 2nd Edn , D. A. McQuarrie, (University Science Books, 2007).
3. Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedmann, (Oxford, 2008).
4. Quantum Chemistry and spectroscopy, Engel & Reid, Pearson (2007)
5. Modern Quantum Chemistry - Introduction to Advanced electronic structure theory - A. Szabo & N. S. Ostlund, (Macmillan, 1982, Dover 1996).
6. Molecular Modeling, Principles and Applications, A. R. Leach, Prentice-Hall, 2001
7. Modern Electronic Structure Theory, D. R. Yarkouy (ed). (World Scientific, 1995)
8. Ab Initio Molecular Orbital Theory, by Hehre, Radom, Schleyer and Pople, (Wiley)
9. Density Functional Theory of Atoms and Molecules, R.G. Parr and W. Yang, Oxford(1989).
10. GAUSSIAN Manual, Gaussian Inc
11. Exploring chemistry with electronic structure methods, Foresman J.B., Frisch A., Gaussian Inc

Course No: CH17408CR
Title: Advanced Electrochemistry and Statistical Mechanics (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Instrumental Methods in Electrochemistry (16 Contact hours)

Fundamentals: Electrode potential and its measurement, standard and formal electrode potentials, three electrode measurements, uncompensated resistance.

Overview of electrode Processes: Faradaic and Non-Faradaic processes, factors affecting electrode reaction rate. Mass transfer: Convection, migration, diffusion, Fick's 1st and 2^{nd} law of diffusion,

Electrochemical Techniques:

Electrophoresis: Factors affecting ion migration, electro-osmosis, theory and applications of capillary electrophoresis.

Potential Step Methods: Chronoamperometry, Chronocoulometry at macro electrodes; theory and applications. Cottrell equation. Controlled-Potential coulometry, Constant-Current coulometric titrations.

Potential Sweep Methods: Linear sweep Voltammetry and Cyclic Voltammetry at macro electrodes theory and applications, Diagnostic criteria of Cyclic Voltammetry.

Unit-II Applied Electrochemistry (16Contacthours)

Electrochemistry of redox enzymes: Direct and mediated electron transfer, Enzyme modified electrodes-challenges and applications. Mechanism and approach to bioelectrosynthesis, examples of bioelectro synthesis-oxidation of alcohols, synthesis of dihydroxy acetone phosphate, site specific oxidation of sugars, reduction of carbonyl compounds, hydrogenation.

Energy storage devices: Desirable characteristics of energy storage devices, Discharge plot, Ragone plot. Batteries: Measures of battery performance. Classical batteries (Lead Acid, Nickel-Cadmium, Zinc-Mangenese dioxide). Modern batteries (Zinc-Air, Nickel-Metal Hydride, Lithium Ion Batteries), Supercapacitors.

Fuel cells, types of fuel Cells, basic fuel cell operation, kinetics of fuel cell reactions. Alkaline, Phosphoric acid, Polymer Electrolyte membrane and direct MeOH fuel cell, biofuel cells.

Unit-III Classical Statistical Mechanics and Ensemble concept (16 Contact hours)

Equations of Motion; Newton, Lagrange and Hamiltonian. Classical partition function, phase space and the Liouville equation, Kinetic theory of gases, equi-partition of energy, Maxwell's velocity distribution.

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. Statistical Mechanical treatment of imperfect gases. Virial equation of state from grand

partition function, virial coefficients in the classical limit, second and third virial coefficients.

Unit-IV Applied Statistical Mechanics (16 Contact hours)

Quantum Statistics: Fermi-Dirac and Boson-Einstein statistics, Nuclear spin statistics, symmetry and nuclear spin, Ortho and Para nuclear spin states, Ortho and Para Hydrogen and Deuterium, CO.

Application of grand partition function to Boson-Einstein and Fermi-Dirac statistics. Ideal Fermi-Dirac gas: Electrons in metals, Ideal Photon gas: Black body radiation, influence of wavelength for the Planck distribution, Bose-Einstein condensation.

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. Electrochemical Methods Fundamentals and Applications, 2ndEdition, Allen J.Bard, Larry R. Faulkner, John Wiley and Sons, INC.
2. Physical Electrochemistry-Principles, Methods and Applications, Israel Rubinstein (Ed.) Marcel Dekker, Inc. New York.
3. Understanding Voltammetry, 2nd Edition, Imperial College Press.
4. Elements of Molecular and Biomolecular Electrochemistry, Jean-Michel Saveant, Wiley-Interscience.
5. Electrochemistry, 2nd Edition, Carl H. Hamann, Andrew Hammett, Wolf Vielstich,Wiley-VCH.
6. Modern Electrochemistry 2B, 2nd Edition, J. O`M. Bockris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.
7. Statistical Thermodynamics, M. C.Gupta ,(NewAgeInternational,1993).
8. Statistical Thermodynamics-Fundamentals and Applications, N.M. Laurendeau, Cambridge University Press, 2005.
9. Statistical Mechanics, D.A. McQuarrie, (Viva,2003).
10. Introduction to Statistical Thermodynamics, Chandler, (OUP, 1987).
11. Statistical Thermodynamics and Kinetic Theory, C. E. Hecht, (Dover,1990).
12. Statistical Mechanics –Principles and Applications, Hill, Dover, 1987.
13. Statistical Thermodynamics for Chemists, A. Ben-Naim, (Plenum, 1992).
14. An introduction to Statistical Thermodynamics, Hill, (Addison-wesley,1987).

Course No: CH17409CR
Title: Chemistry of Materials (04 Credits)

***Max. Marks:** 100* — ***Duration:** 64 Contact hours*
***Ist Unit Exam:** 25 marks* — ***IInd Unit Exam:** 25 marks*
***End Term Exam (units III & IV):** 50 Marks*

Unit-I Surfactant mixtures, Stimuli responsive surfactants and block copolymers (16 Contact hours)

Surfactant-Surfactant Interactions: Mixed micelle formation, mixed monolayer formation, synergism, Clint and Rubingh's models of mixed micelle formation**.** Importance and practical applications of mixed surfactant systems.

Stimuli-Responsive Surfactants: Introduction and applications: Biosurfactants, redox, photochromic, thermoreversible, pH-sensitive, cleavable and magnetic surfactants.

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

Unit-II Hydrogels and microemulsions (16 Contact hours)

Hydrogels: Introduction, Types of Hydrogels, Preparation, Properties and characterization of Hydrogels, Biomedical applications of Hydrogels.

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

Unit-III Langmuir Blodgett Films, Liquid crystals and Fullerenes (16 Contact hours)

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.

Fullerenes: Fullerenes- History, bonding, properties, doped fullerenes, fullerenes as superconductors and fullerene related compounds (carbon nanotubes).

Unit-IV Optical materials and Ionic conductors (16 Contact hours)

Optical materials: Luminesence and phosphors. Lasers – general principle of lasing action, Ruby laser, Neodymium-YAG lasers, semiconducing lasers and quantum dot lasers. Nonlinear optical effects, second and third order harmonic generation, nonlinear optical materials.

Ionic Conductors: Introduction to ionic conduction and mechanism. Types of ionic conductors, mechanism of ionic conduction, interstitial jumps (Frenkel); vacancy

mechanism. Super-ionic conductors: Diffusion and transition superionic conductors and mechanism of conduction in superionic conductors; examples and applications of ionic conductors.

Books Recommended:

1. M. J. Rosen, J. T. Kunjappu, “Surfactants and Interfacial Phenomena”, John Wiley & Sons, New York, 4th Edition, 2012.
2. R. D. Vold and M. J. Vold, “Colloid and Interface Chemistry”, Addison-wesley, 1982.
3. .D. Y. Meyer, “Surfaces, Interfaces and Colloid”, VCH Publishers, Inc. 1991.
4. Jonsson, Lindmann, Homberg and Kronberg, “Surfactants and polymers in aqueous solution”, John Wiley and sons, 1998.
5. D. Fennell Evans, H. Wennerstrom, “The Colloidal Domain where physics, chemistry, biology and technology meet” VCH, New York, 1994.
6. Robert J. Hunter, “Foundations of Colloid Science”, Oxford University Press, New York, 2007.
7. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
8. I. W. Hamley, The Physics of Block Copolymers (Oxford University Press, Oxford, 1998.
9. N. Hadijichristidis, S. Pispas and G. A. Floudas Block Copolymers (Wiley, New York, 2003).
10. Introduction to Solids, Azaroff, Tata McGraw,1993.
11. SolidState Chemistry and its Applications, West, Wiley,1989.
12. The Physical Chemistry of Solids, Borg, Biens, Academic press, 1992.
13. Solid State Physics, N. W. Ashcroft and N. D. Mermin, Saunders college, 2001
14. Principles of Solid State, H. V. Keer, Wiley Eastern.
15. The Physics and Chemistry of materials, J.I. Gersten, F.W. Smith, John Wiley and sons, Inc. 2001.
16. Microemulsions: Background, New Concepts, Applications, Perspectives, C. Stubenrauch, Blackwell Publishing Ltd, 2009.
17. M. Sirousazar, M. Foroug, K. Farhad, Y. Shaabani and R. Molaei, Hydrogels: Properties, Preparation, Characterization and Biomedical, Applications in Tissue Engineering, Drug, Delivery and Wound Care, IN Advanced Healthcare Materials, Wiley online Library, 2014.

Course No: CH17410DCE
Title: Advanced Laboratory Course in Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *75 Marks.* ***Internal Assessment****: 25 Marks*

A: - Inorganic Preparations: (5 Experiments)

- Preparation of tetraamminecarbonatocobalt (III) nitrate and its conversion to pentaamminecholorocobalt (III) chloride.
- Preparation of trans dicholoro bis (ethylenediamine) cobalt (III) chloride and its conversion to cis-isomer.
- Preparation of tris (ethylenediamine) nickel (II) chloride dihydrate and its conversion to bis (ethylenediamine) nickel (II) chloride.
- Preparation of bis (acetylacetonato) copper (II) dihydrate.
- Preparation of pentaamminecholorocobalt (III) chloride and study of Linkage isomers by its conversion to pentaamminenitritocobalt (III) chloride and to nitro isomer followed by IR Characterization.

B:- Total analysis of a Coordination compound for determination of various components present.

(1- Experiment)

C: - Separation by Column Chromatography and Estimations: (5 Experiments)

- Separation of Permanganate and Bichromate ions on Alumina column and their Estimation from Beer Law plots.
- Determination of lonisable chloride in a Complex by cation exchange column (separation followed by Mohr's titration of elute for estimation).
- Separation of Cobalt (II) and Nickel (II) on anion exchange column followed by estimation through EDTA titrations.
- Separation of two Cobalt (III) complexes viz $[Co(NH_3)_6]Cl_3$ and $[Co(NH_3)_5Cl]Cl_2$ on Silica column.
- Ion exchange separation of Hydration / ionization isomers of Chromium (III) Chloride ($CrCl_3$).

D: - Potentiometric Titrations: (6 Experiments)

- Standardization of an Iron (ii) solution with a standard dichromate solution over Pt & Calomel assembly.
- Determination of purity of Ce (IV) Sulphate with a standard Iron (II) solution over Pt & Calomel assembly.
- Estimation of Iodide with Standard $AgNO_3$ over Pt & Calomel assembly using I^- \ I2 redox couple.
- Simultaneous determinations of Chloride and Iodide ions with Standard $AgNO_3$ over Ag-Glass electrode assembly.
- Determination of the purity of $[Co(NH_3)_5Cl]Cl_2$ over Ag-Glass electrode assembly.
- Complexometric titration for determination of Ferro cyanide with standard Zinc (ii) solution and inorder to establish the composition of the complex $K_2Zn_3[Fe(CN)_6]_2$

E: - pH-metric Titrations: (2 Experiments)

- Quantitative analysis of Chromate Dichromate mixture by pH Titration.
- Purity of Acetyl Salicylic acid (Asprin) in a commercial tablet by pH Titration.

F: - Conductometric Titrations: (2 Experiments)

- To determine the solubility and solubility product of a sparingly soluble salt ($BaSO_4$) in water.
- To determine the basicity of sodium potassium tartarate by Conductometric method.

G:- Spectrophotometry: (5 Experiments)

- Determination of Iron (II) with 1,10-Phenanthroline.
- Determination of Phosphate by Molybdenum blue method.
- Determination of formula of Iron (III) thiocyanate complex by Job's Continuous variation method.
- Determination of composition of Iron (II)—2,2-bipyridyl complex by Mole ratio method.
- Determination of rate of Aquation of complex $[Co(NH_3)_5Cl]Cl_2$ in acidic medium.

H: - Flame Photometry: (2 Experiments)

- Simultaneous determination of Sodium and Potassium in the given mixture.
- Determination of Cadmium and Magnesium in tap water.

Books Recommended:

- Vogel's quantitative analysis 6 Edn. Mendham, Denny; Pearson Education 2002
- Synthesis and Technique in Inorganic chemistry , G. S.Girlomi; R.J. Angleci 3rd edn.; University Science Books.
- Synthesis and characterization of Inorganic compounds W.AJolly
- Inorganic syntheses Vols II, VI Academic Press.
- Experimental Inorganic / Physical Chemistry ; Mounir A. Malati Horwood/1999.
- Quantitative Chemical Analysis ; 5th edn.; Harris ; Freeman ; 1999.
- Advanced Practical Inorganic Chemistry ; Adams ; Raynor, Wiley ; 1995.
- Advanced Experimental Inorganic Chemistry ; Ayodha Singh ; Campus Books 2002.

Course No: CH17411DCE
Title: Advanced Laboratory Course in Organic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *75 Marks.* ***Internal Assessment****: 25 Marks*

1. **Multistep synthesis of drugs/ organic coinpouiuls involving name reactions**
   (1) Synthesis oflocal 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.
2. **Extraction/Estimation of Organic compounds from Natural sources**
   (1) Isolation of lycopene and β-carotene from tomato and their characterization using *uv*- spectroscopy.
   (2) Isolation of limonene from its natural source and physicochemical analysis.
   (3) Assay of Belladona for Hyoscyamine.
   (4) Assay of lemon from citric acid and vitamin-C
   (5) Isolation of cholesterol from gallstone
   (6) Assay of coke (soft drink)
3. **Column Chromatography**
   Separation of two component solid mixture. Identification of separated components using physical, chemical and spectral techniques.
4. **Spcctrophotomctric estimation** (UV/visible)
   (1) Vitamin-C (Ascorbic acid)
   (2) Caffeine from tea.
   (3) Cholesterol
   (4) Aspirin
5. **Elcctrophoresis/ Paper chromatography**
   Separation and identification of aminoacids by elcctrophoresis / Paper chromatography.
6. **Spcctroscopy**
   Identification of Organic compounds through interpretation of their spectra (UV, IR, PMR, CMR and Mass. Spectra to be provided).

Books Recommended :

1. Comprehensive Practical Organic Chemistry, V.K. Ahluwalia, Renu Aggarwal (Univ. Press India Limited -2000).
2. Vogel's Text Book of Practical Organic Chemistry, B.S.Furniss, A. J. Hannaford (AWL 5^{th} Ed.-1998).
3. Organic Laboratory Techniques , Donald .C. Pavia, Gary . M. Lampman (SCP 3rdEd.-1999)
4. Experiment Organic Chemistry, John.C. Gilbert., Stephen.F.Martin (SCP -1998)
5. Advanced Practical Organic Chemistry Vol. II, Jag Mohan (Himalaya Pub. House First Ed.-1992.

Course No: CH17412DCE
Title: Advanced Laboratory Course in Physical Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *75 Marks.* ***Internal Assessment****: 25 Marks*

A. Tensiometry

1. Investigation of variation of surface tension of n-butanol and sodium chloride solutions with concentration and hence determination of their surface excess concentrations using Gibb's Adsorption Isotherm.
2. Determination of CMC value of a detergent using tensiometry.

B. Cryoscopy

1. Investigation of variation of freezing point depression with concentration & determination of molecular mass.
2. Determination of the degree of dissociation of a salt/weak acid in solution.
3. Determination of activity co-efficient from freezing point measurements.

C. Spectrophotometry

1. To study the complexation reaction between Fe(III) & salicylic acid.
2. Determination of pK value of an indicator.

D. Spectrofluorometry

1. To determine the rate constant for fluorescence quenching of anthracene or perylene by CCl_4 in ethanol.
2. Using pyrene as probe determine the cmc of a surfactant and site of solubilization of pyrene in the micelle through spectrofluorometry.

E. Potentiometry

1. Precipitation titration of KCl, KBr, KI and their mixture with $AgNO_3$
2. Thermodynamics of a chemical reaction by EMF-method.
3. Determination of (a) Standard electrode potential & (b) Activity Coefficient.

F. Conductometry

1. Verification of Debye-Huckel-Onsagar law.
2. Precipitation titration of $BaCl_2$ and K_2SO_4/ $(NH_4)_2SO_4$
3. Estimation of the concentrations of H_2SO_4, CH_3COOH and $CuSO_4$ in a mixture.

G. Dynamic Electrochemistry

1. To estimate the surface area of a working electrode through chronoamperometry and chronocoulometry.
2. Using Cyclic Voltammetry to determine the formal potential and diffusion coefficient of $[Fe(CN)_6]^{3-}$.
3. Use cyclic voltammetry to determine the concentration of acetaminophen in a given sample.

H. Kinetics

1. Kinetic Investigation of BZ-Oscillatory reaction.
2. Kinetic study of enzyme catalyzed reaction (effect of pH and Temperature).

I. Viscometry and densitometery

1. Determination of Mol. Mass of a Polymer (Polyv inyl alcohol) using viscosity method.
2. To explore the nature of chemical bonding (head-head and Head tail linkage of monomers) in polyvinyl alcohol using Viscometry.
3. Determination of partial molar volume of sodium chloride solutions as a function of concentration from density measurements.

Books Recommended

1. Practical Physical Chemistry --- Findley revised by Kitchner.(Longman, 1971)
2. Experimental Physical Chemistry, A. M. Halpern, G. C. McBane, (Freeman, 2006)
3. Experiments in Physical Chemistry, 5th ed. --- Schoemaker et al. (MGH, 2003)
4. Experimental Electrochemistry---R. Holze (Wiley-VCH, 2009).

Course No: CH17413DCE
Title: Supramolecular Chemistry (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Supramolecular Interactions (08 Contact hours)

Definition and Development of Supramoleclar Chemistry. Nature of Supramolecular Interactions.

Hard Soft Acid Base Concept- Concept, Classification, Symbiosis. Utility in drug design and molecular recognition. Soft Ligands for Soft Metal Ions-Mixed Crown Ethers and Mixed Cryptands.

Unit-II Supramolecular Receptors (08 Contact hours)

Cation Receptors: Supramolecular Cation Coordination Chemistry, EDTA- The Supramolecular Host. Introductory account of Cation Receptors - Podands, Corands, Cryptands, Spherands and Calixarenes.

Anion Receptors: Scope and Challenges, Anion Hydrophobicity-Hofmeister Series, Introductory Account of Anion Receptors - Cyclophanes, Pyrolles, Azacrowns and Metal Based receptors. Hydride Sponge and Anticrowns.

Ion-Pair Receptors: Concept and Significance

Unit-III Crystal engineering and Supramolecular Motiffs (08 Contact hours)

Crystal Engineering: Introduction, Tectons and Synthons. Hydrogen Bond- Introduction, Criteria

Nature and Importance.

Self Assembly: Scope and Objectives. Concepts and Classification. Introductory Account of Coordination Capsules, Catenenes, Rotaxenes and Molecular Knots.

Unit-IV Network Solids and Molecular Devices (08 Contact hours)

Network Solids: Concepts and Classification, Network Topology. Zeolites: Structure, utility and limitations. Metal Organic Frameworks-Introduction and application in catalysis and Gas storage.

Molecular Devices**:** Philosophy of Molecular Devices, Photophysical Fundamentals and Mechanism of Energy and Electron Transfer, Introductory Account of Molecular Wires, Molecular Switches and Molecular Motors.

Books 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, Ist 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. Chemical Reviews. Vol. 115, Issue 15, year **2015**, Pages 6999-8156
8. Introduction: Supramolecular Chemistry. F. Huang and E. V. Anslyn. Chem. Rev. **2015**, 115, 6999−7000.
9. Supramolecular materials. D. B. Amabilino, D. K. Smith and J. W. Steed. Chem. Soc. Rev., **2017**, 46, 2404—2420
10. A Bond by Other Name. G. R. Desiraju. Angew. Chem. Int. Ed. **2011**, 50, 52-59.
11. The Weak Hydrogen Bond: In Structural Chemistry and Biology. G. Desiraju, T. Steiner. **Oxford, IUCr Monograph on Crystallography**.

Course No: CH17414DCE
Title: Designing Organic Synthesis (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I (A) Oxidative and Reductive Processes in Organic Synthesis (8 Contact hours)

Oxidation**:** Introduction, Aromatisation of cycloalkanes and alkenes using metal catalysts and DDQ. Oxidation of Alcohols using chromic acid, DCC and Swern reagent. Oppenaur oxidation. Oxidation of ketones. Oxidation at activated carbon-hydrogen bond. Oxidation with Selenium dioxide. Prevost hydroxylation and its modification by Woodward.

Reduction**:** lntroduction. Reduction of Alkenes, Alkynes and Aromatic rings.

Reduction of carbonyl compounds: Clemmensen and Wolf-Kishner reductions. Reductions using $LiAlH_4$ and $NaBH_4$ Bouveault-Blanc reduction. Reduction of Epoxides, Nitro, Nitroso, Azo and Oxime groups. Reductions using Tributyl Tin Hydride.

(B) Protection and Interconversion of Functional Groups (8 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-II 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, α, β-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; Verlage VCH;1986.
3. Principles of Organic Synthesis 2nd edn;. R. O. C. Norman; Chapman and Hall; 1978.
4. Advanced Organic Chemistry Part B, 5th edn.; F. A. Carey and R.J Sundberg ; Springer; 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, 6lh Ed., J. March,; Wiley; 2012.
9. Organic Synthesis- The disconnection Approach; Sturat Warren; Wiley; 2013

Course No: CH17415DCE
Title: Computational Chemistry (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I

(a) Numerical solution of equations (8 Contact hours)

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

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

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

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

(b) Numerical differentiation and integration (8 Contact hours)

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

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

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

Unit-II

(a) Interpolation and Curve Fitting (8 Contact hours)

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

Lagrange's interpolation method, Newton's divided differences, Cubic spline, piece wise interpolation.

Least squares approximation, linear and quadratic.

(b) Use of Mathematica/Scilab for numerical solution of problems(8 Contact hours)

The mathematica package will be used for the solution of problems covered under the above three units.

Books Recommended

1. Data Reduction & Error Analysis, Bevington& Robinson, (McGraw-Hill, 2003)
2. Computational Chemistry, A. C. Norris, (Wiley.)
3. Computer Software Applications in Chemistry - P. C. Jurs, (John Wiley, 1996.)
4. Numerical Methods for Scientists and Engineers, H. M. Antie, (TMH,).
5. Numerical Recipes in Fortran/C, W.H. Press et al., (CUP,1992)
6. Applied Numerical Analysis, Gerald &Wheatly, (Pearson Education, 2002)
7. Mathematical Methods for Scientists and Engineers, D.A. McQuarie, Viva Books, 1st Ed., 2009.
8. Mathematica Manual.

Course No: CH17416DCE
Title: Seminar (02 Credits)

Presentation by a candidate on any topic chosen in consultation with the teacher incharge.

(25 Marks)

Manuscript (on the topic) submission (25 Marks)

Course No: CH17417GE

Title: Synthetic Polymers and their Applications (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*

Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

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

Course No: CH17418GE
Title: Novel Materials (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

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

Block Copolymers: Introduction: classification, micellization of diblock 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, photoconductivity and sensors.

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

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

Luminesence and phosphors. Lasers - general principle of lasing action, Ruby laser, semiconducing 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 Nanofluids 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, Jeremy Ramsden and Ventus Publishing ApS, 2009.

Course No: CH17419OE
Title: Food Chemistry (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

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_2, 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; 3rd Ed.; Marcel Dekker, Inc. NY; 2005.
2. Food: The Chemistry of its components; T.P. Coultate; 3rd 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; 2nd ed.; Springer International Edition; 2005.

Course No: CH17101CR
Title: Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Stereochemistry and Bonding in the Compounds of Main Group Elements (16 Contact hours)

Valence bond theory: Energy changes taking place during the formation of diatomic molecules; factors affecting the combined wave function. Bent's rule and energetics of hybridization.

Resonance: Conditions, resonance energy and examples of some inorganic molecules/ions.

Odd Electron Bonds: Types, properties and molecular orbital treatment.

VSEPR: Recapitulation of assumptions, shapes of trigonal bypyramidal, octahedral and pentagonal bipyramidal molecules / ions. (PCl_5, VO_3^-, SF_6, $[SiF_6]^{2-}$, $[PbCl_6]^{2-}$ and IF_7). Limitations of VSEPR theory.

Molecular orbital theory: Salient features, variation of electron density with internuclear distance. Relative order of energy levels and molecular orbital diagrams of some heterodiatomic molecules /ions. Molecular orbital diagram of polyatomic molecules / ions.

Delocalized Molecular Orbitals: Butadiene, cyclopentadiene and benzene.

Detection of Hydrogen Bond: UV-VIS, IR and X-ray. Importance of hydrogen bonding.

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

Stepwise and overall formation constants. Inert & labile complexes. Stability of uncommon oxidation states.

Metal Chelates: Characteristics, Chelate effect and the factors affecting stability of metal chelates.

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-III Bonding 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 ML6; Effect of pi-bonding. Molecular orbital and energy level diagram for bonding in Ferrocene, Square-planar and Tetrahedral complexes.

Unit-IV Pi-acid Metal Complexes (16 Contact hours)

Transition Metal Carbonyls: Carbon monoxide as ligand, synthesis, reactions, structures and bonding of mono- and poly-nuclear carbonyls. Vibrational spectra of metal carbonyls for structural diagnosis.

Prepration, reactions, structure and bonding of transition metal nitrosyls, dinitrogen and dioxygen complexes.

Tertiary phosphine as ligand.

Books Recommended

1. Principles of Inorganic Chemistry; 1st edn.; Brain W. Pfennig; Wiley; 2015.
2. Advanced Inorganic Chemistry; 5th. and 6th edn; F.A. Cotton , G. Wilkinson; Wiley; 1998/1999.
3. Inorganic Chemistry; 4th edn; J. E. Huheey; E. A. Keiter; Harper Collins; 2009.
4. Inorganic Chemistry; G. Wulfsberg; Viva; 2002.
5. Chemistry of the Elements; 2nd edn; N. N. Greenwood, A. Earnshaw; Butterworth; 1997.
6. Inorganic Chemistry; 3rd edn; D. F. Shriver; P. W. Atkins; Oxford; 1999.
7. Inorganic Chemistry; K.F. Purcell, J.C Kotz; Saunders; 1977.
8. Coordination Chemistry; D. Banerjea; Tata McGraw Hill; 1993.

Course No: CH17102CR
Title: Organic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Delocalized Chemical bonding (16 Contact hours)

Overview: Inductive effect. Conjugation, Cross conjugation, Hyperconjugation–Isovalent and sacrificial hyperconjugations, Acids / Bases, Nucleophiles and Electrophiles. Resonance, Rules for writing resonance structures, Steric inhibition of resonance.

Tautomerism: Different types including valence 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.

Unit-II Reactive Intermediates and Determination of Reaction Mechanism (16 Contact hours)

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

Determination of Reaction Mechanism: Reaction Mechanism & Types of reactions. Determining reaction mechanism: Structure of Product, Transition states & Intermediates (Hammond postulate). Catalysis including acid and base catalysis, Specific acid and base catalysis. Fate of individual atoms (Isotope Labeling). Stereochemical course of reaction. Thermodynamic and kinetic evidences. Correlation of structure – reactivity.

Unit-III Stereochemistry: (16 Contact hours)

Chirality: Introduction, Chirality due to chiral centre. Molecules with more than one Chiral centres, Threo and erythro isomers. Convention for of assigning D, L & R, S configurations. Optical activity due to chiral axis, chiral plane and helicity. Chirality involving atoms other than carbon. Chirality in metallic complexes. Enantiotopic and diastereotopic atoms, groups and faces.

Asymmetric Synthesis: Introduction and principle of asymmetric synthesism. Principal categories of asymmetric synthesis. Use of chiral substrates. Diastero-selectivity in Aldol reactions. Sterospecificity and steroselectivity of enzymes.

Confirmations: Origin of conformational energy. Angle and Pitzer strain. Conformational analysis of cycloalkanes, and decalines. Effect of conformation on reactivity in acyclic and cyclic systems. Conformation of sugars & anomeric effect. Conformation of cyclohexene, cyclohexanones and bicycloheptane – a bridged system.

Unit-IV Aliphatic Nucleophilic Substitutions : **(16 Contact hours)**

Mechanism and stereochemical implications of S_N2, S_N1, S_Ni and Neighbouring Group Participation (by π and σ-bonds) reactions. Comparison of S_N1 and S_N2 reactions. Effect of substrate structure, attacking nucleophile, leaving group and solvent on the rates of S_N1 and S_N2 reactions. Mixed S_N1 and S_N2 reactions. Nucleophilic substitution at allylic, benzylic, aliphatic trigonal and vinylic carbons. Nucleophilic substitution in alcohols, Mitsunobu reactions. Nucleophilic substitutions on other elements. Functional group transformation using S_N2 reactions in organic synthesis. Nucleophilic substitutions in biological systems.

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

Aliphatic Electrophilic Substitutions: General mechanism of S_E1, S_E2 and S_Ei reactions. Mechanisms of reactions involving migration of double bond. Effect of substrate, leaving group and solvent on reactivity. Stork-Enamine reaction.

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 3rd Ed., S.M. Mukherjee and S.P. Singh. (Macmillan-1998).
4. Stereochemistry of Organic Compounds 2nd Ed., D. Nasipuri. (New Age Inter.- 2008)
5. Stereochemistry of Carbon Compounds - E.L.Eliel. (TMH -2007)
6. Stereochemistry of Organic Compounds 7th Ed. - P.S. Kalsi. (New Age Inter.- 2012).
7. Organic Chemistry - 2nd Ed., J. Hornback. (Brooks/Cole- 2006,
8. Organic Chemistry, 5th Ed., John McMurry. (Brooks/Cole-2000).
9. Advanced Organic Chemistry, 5th Ed., F.A Carey & R.J Sundberg (Springer-2007).
10. Organic Chemistry, 2nd Ed., Jonathan Clayden (OUP-2012)
11. Organic Chemistry, 11th Ed., Solomons, T.W.G., (Wiley-2015).

Course No: CH17103CR
Title: Physical Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

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)

Theories of Chemical Reactions: Activated complex theory of reaction rates, statistical & thermodynamic formulations, comparison with collision theory. Theories of unimolecular reactions (Lindman, Hinshelwood , RRK and RRKM theories), Introduction to potential energy surfaces.

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

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

Unit-IV Chemical kinetics-II **(16 Contact hours)**

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

Reactions in solutions: Diffusion controlled reactions (partial & full microscopic diffusion control), Ionic Reactions; Single & double sphere models of ionic reactions.

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

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

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. CH17104DCE
Title: Laboratory Course in Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *75 Marks.* ***Internal Assessment****: 25 Marks*

I. Preparation of Coordination compounds of Transition metals:

1. Theoretical appraise of first row Transition metal Coordination Chemistry.
2. Synthesis as a Laboratory Technique (Concepts, Calculations and Design of Synthetic procedures).
3. Selected preparations of the following coordination compounds with the specific objectives:

i) Mercurytetrathiocyanatocobaltate(II)	:	To visualize the complexation process.
ii) Tristhioureacopper(I)sulphate monohydrate	:	Insitu generation and Stabilization of unusual oxidation state and re-crystallization /crystal growing
iii) Hexaamminecobalt(III) chloride	:	Multistep synthetic procedure
iv) Trisethylenediaminecobalt(III) chloride	:	Two stage synthesis and aerial oxidation/Resolution of a racemic mixture
v) Ammonium dodeca molbedophosphate	:	Synthesis of a heteroploy metallate/ Bonding and structure.

II. 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.

III.

A. Qualitative Analysis by Semi micro Technique:

Discussion about the analysis scheme. Analytical groups and Group reagents. Scales of Analysis, Skill of semi micro technique. Chemistry involved in separation and identification of less familiar cations by semi micro analysis.

B. Identification of four less familiar cations from different analytical groups with simple and complex combinations:

(i) Group I and II A
(ii) Group I, II A and II B
(iii) Group IIA and II B
(iv) Group I and Group III
(v) Group II B and Group III
(vi) Group III only.

IV. Inorganic Quantitative Analyses:

A. **Gravimetry:**

i) Skill and importance of weighing in Chemistry, Gravimetreric 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.

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) Barium (Ba^{2+}) as BaSO4 and Zinc as $[ZnEDTA]^{2-}$ complex.

iii) Barium (Ba^{2+}) as $BaSO_4$ and Nickel (Ni^{2+}) as $[NiEDTA]^{2-}$ complex.

iv) Nickel (Ni^{2+}) as Ni $(dmg)_2$ complex and Magnesium (Mg^{2+}) as $[Mg\ EDTA]^{2-}$ complex.

v) Copper (Cu^{2+}) as CuSCN and Magnesium (Mg^{2+}) as $[MgEDTA]^{2-}$ complex.

Books Recommended:

1. Advanced Inorganic Chemistry, 5th ed. / 6th 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; 5th edn; Jeffery, Bassett; (ELBS, 1989).
4. Quantitative Analysis; 6th edn; Day, Underwood (Printice Hall, 1993).
5. Analytical Chemistry, 6th Ed; D. Christian, Wiley.
6. Quantitative Analysis; 6th edn; Day, Underwood (Printice Hall, 1993).

Course No: CH17105DCE
Title: Symmetry and Group Theory (02 Credits)

***Max. Marks:** 50* — ***Duration:** 32 Contact hours*
***Ist Unit Exam:** 25 marks* — ***IInd Unit (Term end) Exam:** 25 marks*

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, Symmetry groups and group multiplication tables.

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 Orthoganality Theorm-elementary idea, consequences of the Great Orthogonolity Theorem. Reducible and Irreducible representations, Mullikan symbols for IRS. Character table-construction of character tables for C2v, C3v and C4v point groups.

Applications of group theory to IR and Raman spectroscopy, 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 and Polarity.

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.

Course No: CH17106DCE

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

Max. Marks: *50* | ***Duration:*** *32 Contact hours*

Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

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_2, O_2),

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. Physical Methods for Chemists; R.S.Drago; 2nd edn; Saunders; 1992.
2. Fundamentals of Molecular Spectrsocopy; C.N.Banwell, E.M.Mc Cash; 4th edn; Tata McGrawHill; 1994.
3. Physical chemistry; P. W. Atkins; 6th edition; Oxford University Press; 1998.
4. Electronic Absorption Spectroscopy and related techniques; D N Sathyanarayna; UniversitiesPress.
5. Introductory Raman Spectroscopy; J. R. Ferraro, K. Nakamoto & C. W Brown; 2nd edn; Academic Press 2005.
6. Theory and Applications of Ultraviolet Spectroscopy; H.H.Jaffe, M.Orchin; Wiley; 1962.
7. Molecular Spectroscopy; 1st edn; J L. McHale; Prentice Hall; 1999.
8. Modern Spectroscopy; J.M.Hollas; Wiley; 1987.
9. Basic Principles of Spectroscopy; R.Chang; McGraw Hill; 1971.
10. Structural Methods in Inorganic Chemistry; 2nd edn; E.A.V.Ebsworth, D.W.H.Rankin, S.Cradock; Blackwell; 1991.

Course No: CH17001GE
Title: Chemistry of the Environment (02 Credits)

Max. Marks: *50* — ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Soil and Hydrosphere (16 Contact hours)

Soil: Nature and Composition of soil – Air, Water, Inorganic components, organic matter and humus. Acid – Base and Ion exchange reactions in soil.

Wastes and pollutants in soil: Chemical degradation, photochemical reactions and biodegradation. Desertification, Deforestation and soil erosion.

Hydrosphere: Chemical Composition of Water Bodies: Lakes & rivers, Factors determining composition (thermal stratification, acid-base, pE concept).

Aquatic pollution: Inorganic, Organic, Pesticide, Agricultural, Industrial and Sewage.

Water quality parameters: Dissolved oxygen, Metals, Content of Chloride, Phosphate, Nitrate, and Microorganisms. Water quality standards.

Analytical Methods for determining BOD, DO, COD, and choice of methods for determining metals (As, Cd, Hg, Pb & Se).

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

Unit-II Atmosphere (16 Contact hours)

Chemical Composition of the Atmosphere: Particles, ions, radicals and their formation. Vertical profile of the atmosphere, Heat budget of earth's atmospheric system. Chemical and photochemical reactions in atmosphere, photochemical smog formation.

Oxides of N, C, S and their effects.

Ozone layer: Formation of ozone and mechanism of ozone depletion.

Pollution by chemicals: Chlorofluorocarbons, hydrocarbons and ozone.

Green house effect: Cause, source and impact on global climate.

Consequences of Green house effect and remedial measures.

Acid rain: Chemical aspects, adverse effects and control.

Books Recommended

1. Environmental Chemistry; 5th edn; Colin Baird; Freeman & Co; 2012.
2. Environmental Chemistry; 9th edn.S.E.Manahan; Lewis Publishers;2009
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 pollution; B.K.Sharma & H.Kaur; Goel Publishcrs;1996.
7. Environmental Chemistry; Nigel. J.Bunce; Wurez Publishers; 1991.
8. Environmental Toxicology; Ed.Rose; Gordon & Breach Science Publishers.

Course No: CH17002GE
Title: Surfactants and their Applications (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*

Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Self-Assembly of Surfactants (16 Contact hours)

***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 Systems (16 Contact hours)

a) **Mixed Surfactant systems**: Mixed micelle formation, mixed monolayer formation, synergism, various models of mixed micelle formation(Clint, Rubingh, Motamurra, Blankschtein, and Rubing-Holland models) 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. Characterization of polymer- surfactant systems by various techniques like viscosity, light scattering, spectroscopic and conductance measurements. 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. Physical Chemistry; P.W. Atkins; ELBS; Oxford; 1994.
3. Principles of Colloid and Surface Chemistry; P.C. Heimenz; Marcel Dekker Inc; New York; 1986.
4. Surfactants and Interfacial Phenomena; M. J. Rosen; John Wiley & Sons; New York; 1989.
5. Colloid and Interface Chemistry; R. D. Vold and M. J. Vold; Addison-Wesley; 1982.
6. Surfaces, Interfaces and Colloid; D. Y. Meyer; VCH Publishers; Inc; 1991.
7. Surfactants and polymers in aqueous solution; Jonsson, Lindmann, Homberg and Kronberg; John Wiley and sons; 1998.
8. Advances in Colloid and Polymer Science; B.K.Paul & S.P.Moulik, Current Science,Vol.80,p 990-,2001; Vol.78,p 99,1998.
9. Critical Reviews in Food Science and Nutrition; John Flanagan & Harjinder Singh, ,Vol. 46, pp221-237, 2006.
10. Advanced Drug Delivery Reviews; M. J. Lawrence & G.D.Rees; Vol, 45, p 898, 2000.
11. Energy Fuels; T. N. Dantas, A.A.D, Netoetal; DOI:10.1021/ ef900952y; 2010.

Course No: CH17001OE
Title: Chemistry in Everyday Life (02 Credits)

Max. Marks: *50* — ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit (Term end) Exam:*** *25 marks*

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

(a) Water- An Amazing Chemical Stuff

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)

Course No: CH17201CR
Title: Inorganic Chemistry (04 Credits)

Max. Marks: *100* | ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

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

Energy profile of a reaction; reactivity of metal complexes; inert and labile complexes.

Types of substitution reactions; mechanistic classification of substitution reactions:- Dissociative, Associative, Dissociative conjugate base and Interchange.

Empirical criteria to differentiate the mechanism of substitution reaction.

Substitution in octahedral complexes- Classification of metal ions based on water exchange rates. Metal-complex formation- the Eigen-Wilkins mechanism. Anation reactions.

Hydrolysis Reactions; Simple Acid hydrolysis, Acid catalysed and Base hydrolysis. Stereochemical changes in Octahedral Substitution Reactions.

Substitution reactions without breaking of metal-ligand bond.

Unit-III Mechanism of Ligand Substitution Reactions in Square-Planar complexes:
(16 Contact hours)

Significance of the two-term rate^law, Mechanism, and Steric course of the substitution reactions.

Factors affecting the rate of substitution:- entering and leaving groups; nucleophilicity of entering group and the n_{pt} scale, central metal ion, solvent and the non-leaving groups.

The Trans effect;- Theories, applications in synthesis.

cis-trans isomerization in square planar complexes.

Unit-IV Organo Metallic Compounds (16 Contact hours)

Introduction, Nomenclature, classification and importance of organometallic compounds.

Nomenclature and Classification of Organometallic compounds.

Effective atomic number (18-Valance electron) rule and its significance.

Stability of Organometallic Compounds towards heat, oxidation and hydrolysis.

Preparation, Properties, Structure, bonding and applications of Alkyls and aryls of Li, B and Al.

Synthesis, Structure and bonding in Zeise's Salt.

Homogenous Catalysis using Organometallic Compounds: Catalysis, Terminology of Catalysis and Tolman Catalytic loop;

Oxidative addition, reductive elimination and migration (insertion) reactions.

Hydrogenation and Hydroformation reactions in alkenes.

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. CH17202CR
Title: Organic Chemistry (04 Credits)

Max. Marks: *100* — ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Aromatic Electrophilic Substitution (16 Contact hours)

Overview: Arenium ion mechanism, Sigma and pi – complexes, Energy profile diagram, Effect of leaving group. Orientation and reactivity in mono substituted benzene ring , *Ortho / Para ratio*, Ipso attack.

The Third substitution : Orientation of substitution in benzene ring with more than one substituent. Orientation in other ring systems. Carboxylation of aromatic rings with $COCl_2$ and amidation with NH_2COCl. Reversal of F.C. acylations. 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 mechanism (S_N1, S_NAr, Benzyne and $S_{RN}1$). Structure reactivity relationships. Effect of leaving group and attacking nucleophile. Mechanisms of Von-Richter, Sommelet-Hauser and Smiles rearrangements and Chichibabin reaction.

Free Radical Substitution:

Free radical substitution mechanisms. Mechanisms at an aromatic substrate. Neighbouring Group Assistance in free radical reactions, Reactivity for aliphatic and aromatic substrates. Reactivity in the attacking radical. Effect of solvent on reactivity.

Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sandmeyer reaction, free radical rearrangements and Hunsdiecker reaction.

Unit-II Addition to multiple bonds. (16 Contact hours)

Addition to carbon-oxygen double bonds:

Overview of reactivity carbonyl compounds: Mechanisms of addition of water , hydrogen cyanide, alcohols , amines , organometallic reagents and hydrides to aldehydes and ketones.

Mechanism of Wittig, Mannich , Aldol, Cross Aldol , Cannizarro's , Knoevenagel, Robinson annulation, Claisen, Dickman , Benzoin , Perkin and Stobbes reactions.

Addition to carbon-carbon multiple bonds:

General mechanism, reactivity, orientation and stereochemical implications of additions reactions involving electrophiles, nucleophiles and free radicals. Addition to cyclopropane ring. Hydrogenation of double/triple bonds and aromatic rings. Hydroboration, Ene-reaction, Michael reaction and Sharpless assymetric epoxidation.

Unit-III Molecular Rearrangements (16 Contact hours)

General mechanistic treatment of nucleophilic, electrophilic and free radical rearrangments. Nature of migration and migratory aptitude and memory effect. Detailed study of following rearrangements: Wagner-Meerwein, Pinacol- Pinacolone, Demyanov, Benzil-Benzilic acid, Favorskii, Arndt-Eistert, Neber, Hofmann, Curtius, Lossen, Schmidt, Beckmann, Baeyer-Villiger, Pyne and Dienone - phenol rearrangements.

Unit-IV Pericyclic reactions. (16 Contact hours)

Molecular orbital symmetry, Frontier orbitals of ethene, 1,3- butadiene, 1,3,5-hexatriene and allylic systems. HOMO, LUMO concept, FMO approach. Classification of Pericyclic reactions. Woodward Hofmann rules for the following pericyclic reactions. Cycloadditions: Thermal and Photochemical 2+2 and 4+2 cycloadditions. Suprafacial and antrafacial cycloadditions.

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

Sigmatropic rearrangements: Classification, [1,3], [1,5] and [3,3] sigmatropic shifts. Cope and Claisen rearrangements. Suprafacial and antrafacial shifts of hydrogen atom.

Books Recommended

1. Advanced Organic Chemistry Reactions, Mechanism and Structure, 4th Ed.,Jerry March. (Wiley, 1999).
2. Advanced Organic Chemistry 4th Ed. - F. A. Carey and R. J. Sundberg. (Plenum, 2001).
3. A Guide Book to Mechanism in Organic Chemistry 6th Ed.- Peter Sykes. (Longman, 1996).
4. Structure and Mechanism in Organic Chemistry 2nd Ed. - C. K. Ingold. (CBS, 1994).
5. Modern Organic Reactions 2nd Ed. - H.O. House (Benjamin, 1972)
6. Principles of Organic Synthesis 2nd Ed. - R.O.C. Norman (Chapmann Hall, 1978)
7. Reaction Mechanism in Organic Chemistry 3rd Ed. - S.M. Mykherjee and S.P. Singh. Macmillan, 1998).
8. Organic Chemistry - J. Hornback,pk. (Brooks/Cole, 1998).
9. Fundamentals of Organic Cbemjstry , 5th ed.- Solomons. (Wiley, 1992).
10. Organic Chemistry, 5th Ed.- John McMurry. (Brooks/Cole, 2000).

Course No: CH17203CR
Title: Physical Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I 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.

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.

Ion solvent Interactions*:* Non structural (Born) treatment and an introduction to structural (Ion-dipole, Ion-quadruple) 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.

Unit-III Biophysical Chemistry (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 (synthesis & hydrolysis), Principles of coupled reactions and their importance for living systems.

Biopolymers: Molecular forces and Chemical bonding in Bio-polymers, hydrophobic interactions, structure of proteins, protein folding and unfolding. Biological membranes, phase transitions in biological membranes. Donan effect and transport across biological membranes.

Binding of Ligands and metal Ions to bio-macromolecules, one binding site per macromolecule, n equivalent binding sites per macromolecule, binding of oxygen to myoglobin and hemoglobin.

Unit-IV Statistical Thermodynamics (16 Contact hours)

Concept of distribution, thermodynamic probability and most probable distribution. Sterling approximation. Method of undetermined multipliers.

Distribution Laws: Derivation of Boltzmann distribution law, Bose-Einstein and Fermi-Dirac laws (without derivation) and their comparison with Boltzmann distribution law.

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

Books Recommended:

1. Physical Chemistry –P. W. Atkins, 9th Edition, 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, Lioyd L Lee, World Scientific, 2008.
7. An Introduction to Aqueous Electrolyte Solutions, Margaret Robson Wright, Wiley, 2007.
8. Modern Electrochemistry 1, 2A, 2nd Edition, J. O`M. Bokris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.
9. Physical Chemistry for the Biosciences, Raymond Chang, University Science Books, 2005.
10. Physical Chemistry for the Life Sciences,2nd Edition, Peter Atkins, Julio de Paula, Oxford University Press2015.
11. Statistical Thermodynamics, M.C.Gupta, New Age International, 1993.
12. Statistical Mechanics, Agarwal, Eisner, Wiley, 1991.

Course No: CH17204DCE
Title: Laboratory Course in Organic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *80 Marks.* ***Internal Assessment****: 20 Marks*

1. **Qualitative Analyses of Organic Compounds**
   (i) **Physical Properties:** Physical state, colour, odour, solubility behavior 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, Nitrocompounds and Hydrocarbons.
   (iii) **Preparation and recrystallization of the derivatives of above mentioned group of compounds.**
2. **Separation, Purification and identification of Organic compounds from a three component mixture:**
   (a) **Separation based on solubility in water and organic solvents.**
   (b) **Separation based on Chemical properties:** Solubility in Sodium bicarbonate, Sodium Hydroxide and Hydrochloric acid.
   (c) **Identification of individual components using physico-chemical properties**
3. **Detection of functional groups using IR spectroscopy (spectra to be provided)**
4. **Quantitative Estimation of the following compounds**
   (a) Glucose.
   (b) Glycine
   (c) Acetone
   (d) Phenol.
   (e) Ascorbic acid.

5. Organic Preparations

(a) Acetylation of Cholesterol or salicylic acid.

(b) Oxidation of Cyclohexanol by chromic acid to get adipic acid.

(c) Aldol condensation: Dibenzal acetone and benzaldehyde.

(d) Cannizarro's reaction of 4-Chlorobenzaldelyde.

(e) Aromatic electrophillic substitutions in benzene, benzoic acid or aniline.

(f) Beckman rearrangement starting from acetophenone.

(g) Haloform reaction: Preparation of Iodoform.

Books Recommended:

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

Course No: CH17205DCE
Title: NMR and ESR Spectroscopy (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I NMR Spectroscopy-I (08 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 (T1, T2). Shielding and deshielding of magnetic nuclei. Chemical shift, its measurement and factors influencing chemical shifts; local paramagnetic and diamagnetic shielding, neighboring group anisotropy and ring currents in aromatic systems

Unit-II NMR Spectroscopy-II (08 Contact hours)

Spin- Spin coupling, coupling constants. Examples.
Vicinal coupling and electron correlation. Chemical equivalence and magnetic equivalence.
Fermi contact and Dirac Vector Model. Effect of Chemical exchange on spectra.
Double resonance techniques; spin decoupling, nuclear overhauser enhancement.
Instrumentation; FT-NMR and its advantages. NMR studies of nuclei other than proton – ^{13}C, ^{19}F and ^{31}P.

Unit-III ESR spectroscopy-I (08 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

Unit-IV ESR spectroscopy-II (08 Contact hours)

Fermi contact, Spin polarization effects, Dipolar coupling, Mc Conell equation and calculation of spin densities in inorganic radicals such as $CO_2^{-\bullet}$, $CH_3^{\bullet}$, $BH_3^{-\bullet}$ and $F_2^{-\bullet}$.
Spin orbit coupling and significance of g tensors.
Zero field splitting and Kramer's degeneracy (fine structure),
Advance Applications

Books Recommended

1. Introduction to Spectroscopy; 3rd edn.; D. L. Pavia, G. M. Lampman, G. S. Kriz; Saunders-Thomson learning; 2001.
2. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry; R. V. Parish; Ellis Horwood; 1990.
3. Nuclear Magnetic Resonance; P. J. Hore; Oxford; 1995.
4. Principles of Instrumental Analysis; 4th edn.; D. A. Skoog, J. J. Leary; Saunders; 1992.
5. Physical Methods for Chemists; 2nd edn.; R. S. Drago; Saunders; 1992.
6. Basic Principles of Spectroscopy; R. Chang; McGraw Hill; 1971.
7. Introduction to Magnetic Resonance; A Carrington, A. D. McLachlan; Harper & Row; 1967.
8. NMR and Chemistry; 2nd edn.; J. W. Akitt; Chapman and Hall; 1983.

Course No: CH17206DCE
Title: Solid State Chemistry (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Structure and Theories of Solids (16 Contact hours)

Structure of solids: 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. *S*tructure 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, Colour centres, Dislocations and their types.

Theories of solids:

Free electron theory of metals**:** The Drude Model, Lorentz modification, Sommerfield Model; Fermi-Dirac distribution function, Density of states, electronic heat capacity, Hall effect.

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. 10^{th}, 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: CH17207GE
Title: Metal Ions in Living Systems (02 Credits)

Max. Marks: *50* — ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Alkali and Alkaline Earth Metal-ions in Biosystems (16 Contact hours)

Biomolecules and their Metal Coordination behavior.

Evidence of the presence of metal ions in biological systems (Direct / Indirect). Classification of metals and non-metals according to their action in biological systems.

Essential Elements: Concept of essentiality, criteria and classification of essential elements as per their role in living systems.

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.

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. Dioxygen transport (Haemocyanin).

Zinc in Biosystems: Lewis acid catalyst, Enzyme activator in vitamin B_{12}.

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

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

Antibacterial, Antiviral and Antifungal activities of metal complexes: Labile and Robust metal complexes; probable mechanism of action.

Books Recommended

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

Course No: CH17208GE
Title: Bio-Physical Chemistry (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Bioenergetics & Equilibrium in biological Systems (16 Contact hours)

Relevence of thermodynamics to Biological systems, Biochemists standard state, standard energy changes in biochemical reactions, ATP as energy currency of cell (synthesis & hydrolysis). Principles of coupled reactions and their importance for living systems.

Acid–base Equilibria: pH, pKa & pKb values. Dissociation of Amino-acids, isoelectric point. Buffer solutions, buffer capacity, effect of ionic strength & temperature, maintaining pH of blood.

Electrochemical equilibria: Standard redox potential, half- cell potentials of biological reactions, Nernst Equation.

Biological Membranes, Transport of ions across biological membranes, active and passive transport. Theory of membrane potential.

Unit-II Bio-electrochemistry, Kinetics & Spectroscopy (16 Contact hours)

Electrochemistry of Nerve conduction, medical applications of electrochemistry.

Renaturation of DNA as a second order reaction, Enzyme kinetics, Michaelis-Menton mechanism, competition & inhibition, multisubstrate systems, effect of substrate concentration, temperature and pH.

Fluorescence spectroscopy: Simple theory, excited state properties, florescence quenching, molecular rulers (FRET), single molecule florescence, applications in biological systems.

ORD and CD spectroscopy: Polarization of light and optical rotation, Optical rotatory dispersion and Circular dichroism, Circular dichroism of nucleic acids and proteins.

Books Recommended:

1. Physical Chemistry for life sciences; 2^{nd} edn.; P. W. Atkins and J.D. Paula; Oxford University Press; 2010.
2. Fundamentals of general Biological Chemistry; 4th edn.; John . R. Holum; Wiley; 1990.
3. Principles of biochemistry; 3rd edn.; David. L .Nelson, Michael .M.Cox; Worth Pub.; 2002.
4. Physical Chemistry, Principles and applications in biological systems. 4^{th}edn. Tinoco, Sauer, Wang, Puglisi. Pearson education, 2007.
5. Biophysical Chemistry; 2^{nd}edn.; Alan Cooper; RSC. Publishing; 2011.

Course No: CH17209OE
Title: Chemistry of Bio-molecules (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

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

Oils and Fats: Fatty acids and Triglycerides. Saturated and Unsaturated fatty acids (MUFA and PUFA). Rancidity of Oils & Fats. Absorption of toxic substances by fat.
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.
Minerals: Macro and Micro minerals. Their functions and diseases caused by their deficiencies.

Books Recommended

1. Organic Chemistry; 5^{th} edn;. Vol.2,1.L. Finar (Addison Wesley Longman-2000).
2. Biochemistry, Biotechnology and Clinical Chemistry of Enzymes; Trevor Palmer (EWP). Organic Chemistry by I.L.Finar; Vol. II (ELBS Longamnn).
3. Lehninger's Principles of Bio-chemistry; D.L. Nelson; M.Cox Worth publications; 2000.
4. Introduction to Nucleic Acids and Related Natural Products; Ulbight; Oldborn Press.
5. Chemsitry of Natural Products; S.V. Bhat, B.A. Nagasampagi, M. Siva Kumar. Naroosa Publishing House; New Delhi.

Course No: CH17309OE
Title: Philosophy of Science (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Representation (08 contact hours)

Laws of nature**:** Knowledge**, S**ources of knowledge, The rationalists, The empiricists, The Mathematical knowledge, Synthetic Knowledge, Science as knowledge source, Religion and science The Method of science, Induction versus deduction, Representation and reason, Probabilistic laws, Basic and derived laws,

Realism: Realism and its critics, Instrumentalism, Constructive empiricism, Laws and antirealism, Anti-realism and structure of science.

Unit-II Reason (08 contact hours)

Inductive Scepticism: Theory and observation, Dissolving the problem of Induction, Probability
and scientific inference, Kinds of Probability,

Inductive Knowledge: Reliabilist epistemology, reasoning with induction, Innate epistemic capacities and reasoning about induction, Internalism and justification.

Method and Progress: Methodology of scientific research programmes, Clinical trials and the scientific method, The content of discovery and the context of justification, Science without the scientific method, Method and the development of sciences, Paradigms and Progress.

Unit-III Classical Determinism and Probabilistic world (08 contact hours)

The Classical Mechanics: Mechanistic determinism, General principles; Action at a distance, Electric and magnetic forces, Failures of the classical mechanics;
Atomic structure, problem of radiation.

The birth of modern science**:** The photo-electric effect**,** The atomicity of radiation, Particle wave duality, waves of probability, Uncertainty principle, subject versus object, the fundamental laws of radioactivity, The new Quantum theory, wave mechanics, Diracs Quantum mechanics, The new philosophical principles, the probabilistic reasoning.

Unit-IV The Dawn of Modern Thinking (08 contact hours)

The arrow of Time: From Descarts to quantum theory, the relation of quantum theory to other natural sciences. Language and reality in modern science. The role of modern science in the present development of human thinking.

Books Recommended:

1. Philosophy of science; Alexander Bird; McGill-Queen's University Press.
2. Physics and Philosophy; W. Heisenberg; Harper Perennial Modern Classics.
3. Physics and Philosophy; Sir James Jeans; Cambridge University Press.
4. Reconstruction of religious thought in Islam; Muhammad Iqbal; Adam Publishers & Dodo Press.
5. Philosophy of natural science; Carl G. Hempel**;** Pearson.
6. The philosophy of science; David Papineaus; Oxford University Press.
7. Reality and Representation; David Papineaus; Blackwell Publication.
8. Belief, truth and knowledge; D.M. Armstrong; Cambridge University Press.
9. Modern epistemology; Nicholas Everitt and Alec Fisher; McGraw-Hill Higher Education.
10. The structure of scientific revolution; Thomas S. Kuhn; The University of Chicago Press

Course No: CH17401CR
Title: Organo-Transition Metal Chemistry (04 Credits)

Max. Marks: *100* | ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Sigma Bonded Organometallic Compounds: (16 Contact hours)

Classification, Stability, Comparison to main Organometallic Compounds, Routes of synthesis, Reactions. Decomposition Pathways: Choice, α and β hydrogen transfer. Intramolecular elimination of alkane, Cyclometallation, Stability from bulky substituents, Agostic alkyls, Umpolung.Metal Hydride Complexes: Synthesis, Characterization and Chemical reactions, Non-classical Hydrides (Kubas complexes).

Unit-II Pi-bonded Organometallic Compounds: (16 Contact hours)

Classification, Structure and bonding in Metal- alkene, alkyne, allyl, 1,3-butadiene and Cyclobutadiene Complexes.

Sandwich Compounds: Characteristics; Classification, Synthesis, Reactions, 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.

Unit-III Catalytic Processes involving Transition Metal Organometallic Compounds: (16 Contact hours)

Mechanistic aspects: Oxidative addition, Insertion reactions Reductive elimination and water gas shift reaction (WGSR).

Catalytic mechanism of Hydrogenation, Hydroformylation, Oxidation and Isomerization of alkenes; Olefin metathesis.

Fischer-Tropsch Synthesis and Ziegler Natta polymerization of alkenes.

Asymmeteric and supported Organometallic Catalysis (brief idea)

Unit-IV Fluxional Organometallic Compounds and Synthetic Reactions involving Organo- metallics (16 Contact hours)

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 η^1 Cyclopentadienyls and η^3–allyls.

Stereochemical non rigidity in case of coordination numbers- 4 & 5 (cis-trans, atomic inversion, Berry Pseudorotation).

Synthetic Reactions involving Organo- metallics:

Reactions of coordinated ligands, carbon monoxide, alkyls, alkenes (Green, Mingo’s rules). Activation of small molecules: Carbon monoxide, Carbon dioxide and Alkanes.

Role of organo-iron as synthons, Carbon-Carbon coupling and its reactions (Suzuki and Heck).

Books Recommended:

1. The Organometallic Chemistry of Transition Metals; 2nd edn; Robert. H . Crabtree; Wiley; 1994.
2. Fundamental Transition Metal Organometallic Chemistry; Luke hart; Brooks / Cole; 1985.
3. Organometallic Chemistry; 2nd edn ; Mehrotra & Singh ; New age international 2000
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 press 1983.
9. Reaction Mechanism of Inorganic and Organometallic systems; 2nd edn.; Robert .b. Jordan 1998.
10. Inorganic Chemistry ; 4th edn.; Huheey ; E. Keiter & R. Keiter; Addison-Wesley ;1983
11. Modern Inorganic Chemistry; William. A. Jolly; McGraw Hill; 1985.

Course No: CH17402CR
Title: Photo-Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Basics of Photo-Chemistry (16 Contact hours)

Absorption; mechanism of absorption of light

Transition moment integral, Einstein's treatment, molar integrated absorption intensity, natural radiative lifetime & the calculation of life times.

Excitation; d-d transition, charge transfer & intraligand 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 diagramsdepicting excited states.

Frank Condon principle, shapes of absorption & emission bands.

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

Tools and Technique: Light source, measurement of light intensity, chemical actinometry. Flash photolysis.

Unit-II The Chemistry of Excited State Molecules (16 Contact hours)

Photochemical laws & quantum yield. Kinetics & quantum yield of photo-physical (radiative) and photo-chemical processes. Photochemical processes: primary, secondary, adiabatic & non- adiabatic. Properties of thexi states; Determination of dipole moments & acidity constants of excited state molecules.

Photosubstitution and photo reduction of Co (III) complexes.Photosubstitution reaction of Cr (III) and Rh (III) complexes.

Organometallic-Photochemistry: Reactions of metal carbonyls, cleavage of metal-metal bond.

Unit-III Redox Reactions by Excited Metal Complexes (16 Contact hours)

Energy transfer under conditions of weak and strong interaction. Excited state electron transfer. Marcus-Hush model.Conditions of the excited states to be useful as redox reactants. Photochemical electron transfer, [Ru (bipy)3]2+ and [Os (bipy)3]2+.

Photochemical supramolecular devices: devices for photo-induced energy or electron transfer, Devices for information processing, photo-chemically driven molecular machines.

Unit-IV Solar Energy-Prospects and Challenges (16 Contact hours)

Solar energy storage, solar energy conversion, Metal complex sensitizers and electron relays in photochemical splitting of water, Nitrogen fixation and CO_2 reduction. Inorganic photolithography.

Supramolecular photochemistry in natural systems: photosynthesis, bacterial photosynthesis and artificial photosynthesis.

Books Recommended:

1. Reaction Mechanisms of Inorganic and Organometallic Systems; 2nd edn.; Jordon; Oxford; 1998.
2. Mechanism of Inorganic Reactions; Katakis, Gordon; Wiley; 1987.
3. Inorganic Chemistry; 4* edn; Huheey; Harper & Row; 1990.
4. Mechanism of Inorganic Reactions, 2nd edn, Basalo, Pearson; Wiley Eastern, 1997.
5. Chemistry of Light; Suppan, Royal Society; 1994.
6. Photochemistry, Carol J. Wayne and Richard P. Wayne; Oxford University Press; 1996.
7. Fundamentals of Photochemistry; C Rohatgi, Mukhergi; Wiley Eastern.; 1992
8. Inorganic Photochemistry; J.Chem Edu.;Vol .60, No.10,1983.
9. Applications of Inorganic Photochemistry; J. Chem. Edu.; Vol.74, No 69. 1997.

Course No: CH17403CR
Title: Bio-Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Iron Storage, Transport and Oxygen carriers: (16 Contact hours)

Structure and Coordinating sites in biologically important ligands: Proteins, Nucleotides and Lipids.

The transport mechanism: uniport, symport and antiport.

Ferritin and Transferrin: Structure, Metal binding sites; incorporation and release of iron.

Porphyrins: Introduction, characteristic absorption spectrum and salient characteristics.

Haemoglobin and Myoglobin: Structure, oxygen saturation curves; Mechanism of oxygen transport and storage.Bohr effect and cooperativity in haemoglobin.

Hemerythrin and Hemocyanin: Structure, Metal binding groups and Dioxygen binding. Synthetic oxygen carrier model compounds: Vaska's iridium complex: Cobalt complexes with micro and macrocyclic ligands and Schiff base ligands.

Unit-II Metallo-enzymes and Electron Carriers (16 Contact hours)

Enzyme, Apoenzyme, Coenzyme, Prosthetic group and Metalloenzymes, Mechanism of enzyme action.

Zinc enzymes:- Carboxypeptadiase and Carbonic Anhydrase : Introduction, Structure, Mechanism of action and their model compounds.

Biological chemistry of Molybednum: uptake of Molybednum; oxidation states and redox potentials in enzymes and oxygen atom transfer reactions.

Xanthine oxidase and Aldehyde oxidase: Structure and biological role.

Cobalt in Vitamin B_{12}: Introduction, Structure and Derivatives of B_{12} and mechanism of alkylation reaction. Role of vitamin B_{12}.

Electron Carriers: Rubredoxin & Ferridoxin (Structure and biological role).

Blue Copper proteins: Oxidases and Plastocyanin (Structure and biological role).

Unit-III Metal-ion Induced Toxicity and Chelation Therapy (16 Contact hours)

Toxic levels of different metals. Sources of metal ion poisoning (external sources and internal disorders).

Mechanism of metal ion induced toxicity:- Toxicity of Pb, Cd, Hg, As, and CN- Metal ion promoted Carcinogenesis and probable mechanism of action.

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 Metal Salts and Metal Complexes in Therapeutics (16 Contact hours)

Treatment of essential metal deficiencies: Iron, Copper and Cobalt.Metal salts as anti-acids, antiseptic and diuretics.

Gold compounds and Rhematoid arthiritis.

Anti-Cancer Drugs: cis-Platin and its derivatives. Structure-function relationship.

Complexes of Rhodium, Gold and Cobalt.

Anti-bacterial, Anti-viral and Anti-fungal activities of Metal Complexes: Labile and Robust metal complexes; Probable mechanism of action.

Books Recommended:

1. As listed for Course No. CHM—101 (Inorganic chemistry-M.Sc. 1st Semester! From serial No. 1 to 5.
2. Bio inorganic Chemistry -An introduction; Ochai, Allyn and Bacon; 1977.
3. Inorganic Bio-chemistry—Vol. 1&2; Eichhorn; Elsevier, 1973.
4. Inorganic Aspects of Biological and Organic Chemistry; Hanzilik; Academic; 1976.
5. The Inorganic Chemistry of Biological processes; 2nd edn.; Hughes ; Wiley; 1973.
6. A Text book of Medicinal aspects of Bio inorganic Chemistry; Das; CBS; 1990.
7. The Biological Chemistry of Elements; Frausto de Silva; Williams; Clarenden; 1991.
8. Principles of Bio inorganic Chemistry; Lippard, Berg; Univ. Science Books; 1994.
9. Inorganic Chemistry in Biology; Wilkins C & Wilkins G; Oxford; 1997.
10. Bio inorganic Chemistry ; K. Hussain Reddy; New Age International (P) Ltd; 2005.
11. Metal -Ions in Biochemistry; P. K. Bhattacharya; Narosa Publishing House; 2005.

Course No: CH17404CR
Title: Heterocyclic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Structure and Nomenclature of Heterocyclic compounds (16 Contact hours)

Introduction and significance of heterocycles in day to day life.

Nomenclature of Heterocycles: Monocyclic, bicyclic and polycyclic heterocycles, Hantzsch-Widman and replacement methods of nomenclature.

Structural features: Non-aromatic, aromatic and heteroaeromatic heterocycles.

Tautomerism in heterocycles, Meso-ionic systems.

Spectroscopic properties of heterocycles (UV,Visible and ^{1}HNMR).

Unit-II General Approach to Synthesis of Heterocyclic compounds (16 Contact hours)

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 quinoline, Bischler-Napieralki Isoquinoline,Knorr Pyrrole,Paal-Knorr , Fischer – Indole synthesis.

Unit-III Monocyclic Heterocycles (16 Contact hours)

Structure, Synthesis and Reactions of Oxirane, Thirane, Azetidine, Pyrrole, Furan, Thiophene, Diazenes, Pyrimidines,Pyridine.Chemistry of five membered heterocycles with two heteroatoms like 1,3-Azoles, 1,2- Azoles. Chemistry of Six membered rings like Azines and seven membered heterocycles like Azepine,Oxipene,Thiepins.

Unit-IV Bicyclic Heterocycles (16 Contact hours)

Structure, Synthesis and reactions of Benzo- fused heterocycles like Benzo-pyrrole, Benzo-furan,Benzo-thiophene, Quinoline, Isoquinoline, Chromones, Coumarins, Iso-Coumarins, 2 and 4-benzopyrones, Benzopyryllium salts and purines.

Books Recommended:

1. Heterocyclic Chemistry, 5th Ed. J.A.Joule and K.Mills, (Wiley-2010).
2. Essentials of Organic Chemistry, Paul M Dewick , (Wiley-2006).
3. Heterocyclic Chemistry, J.A. Joule and G.F.Smith , (Chapman and Hall-1996).
4. The Chemistry of Heterocycles Theophil Eicher and Siegfried Hauptmann , (George Thieme Verlag Stutt gart,New York -1995).
5. Heterocyclic Chemistry, Raj K. Bansal, (New Age International Publisher-2006).
6. Heterocyclic Chemistry, R.R.Gupta,M.Kumar,V.Gupta,(Springer-2006).

Course No: CH17405CR
Title: Chemistry of Natural Products (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Terpenoids and Carotenoids (16 Contact hours)

Introduction, classification, general methods of isolation, separation.

Essential oils: Separation using Gas Liquid Chromatography and High Performance Liquid Chromatography. Physical, chemical and spectral methods of structure elucidation.

Structure determination, stereochemistry and synthesis of α-terpineol, abietic acid and β-carotene.

Unit-II Alkaloids (16 Contact hours)

Introduction, classification, nomenclature, qualitative tests, pharmaceutical applications and general methods of isolation. Physical, Chemical & Spectral methods of structure elucidation.

Stereochemistry, synthesis and biosynthesis of Quinine, Morphine and Reserpine.

Unit-III Steroids (16 Contact hours)

Introduction, nomenclature, classification & stereochemistry. Physical, Chemical & Spectral methods of characterization. Qualitative tests.

Cholesterol: Isolation, clinical significance, chemical properties, structure elucidation, total synthesis & relationship with bile acids.

Sex hormones: Introduction, isolation, clinical & commercial significance, color reactions, structure determination and partial synthesis of Oesterone, Androsterone, Testosterone and Progesterone.

Glucocorticoids & Mineral Corticoids: Introduction and partial synthesis of Cortisone, aldosterone and synthesis of cholecalciferol.

Unit-IV Natural Plant Pigments and Porphyrins (16 Contact hours)

Introduction, classification, physical, chemical, degradative and spectral methods of structure determination and biosynthesis (Acetate and Shikimic acid pathway)

Flavonoids: Isolation, separation and quantification. Antioxidant activity of flavonoids. Robinson's synthesis, Baker Venketraman synthesis, Kostanecki synthesis of flavanone and Flavanol.

Isolation, structure determination and synthesis of Cyanidin, Chrysin, Quercitin & Genestein.

Porphyrins: Structure determination and total synthesis of haemoglobin. Structural comparison with chlorophyll.

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. New Trends in Natural Product Chemistry, Atta-ur-Rahman (Harward Academic Press).
4. Chemistry of Natural Products, N.R. Krishnaswamy (University Press-1999).
5. Flavanoids; Oyvind M. Andersen and Kenneth R. Markhan. (Taylor & Francis -2006)

Course No: CH17406CR
Title: Bio-Organic and Medicinal Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

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

Vitamins:_ Source, structure and synthesis of vitamins – Vitamin A, Vitamin B-Complex (Thiamine riboflavin, folic acid); Vitamin B-12 (Structure only) Vitamin C, E, K, H and D.

Prostaglandins : Introduction and nomenclature, approaches to prostaglandin synthesis, cyclo-hexane, precursors-Woodward synthesis of PGF2a. Cyclo-heptane precursors - Corey's synthesis of prostoglandin's E & F.Their relationship with oxygenase I and II.

Nucleic Acids: Structure of nucleotide, nucleosides, RNA and DNA, role of nucleic acids in protein synthesis, genetic code and heredity. DNA finger printing

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

Enzymes : Introduction, nomenclature & classification.. Activation & inhibhion of enzymes. Mechanism of enzyme action- Fischer lock and key, koshlands induced fit hypothesis, displacement reactions & coupling of ATP. Enzyme mechanism of chymotrypsin lysozyme & carboxypeptidase.

Co-Enzymes: Cofactors derived from vitamins, coenzymes, prosthetic groups. Apoenzyme. Structure , biological function and mechanism of reactions catalsed by co-enzymes: coenzyme A, thiamine pyrophosphate. pyridoxal phosphate, NAD+, NADP+, FMN, FAD and Lipoic acid.

Unit-III **(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, carbonylic, thiols sulphides groups and introdction/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. Lipophillic constant, Hamett constant, steric parameters and Hansch analysis.

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

Antibiotics: Classifications-structural and mechanistic, cell wall biosynthesis inhibitors, protein synthesis inhibitors. Pencillins-classification and structures. Synthesis of Pencillins, V, G, chloroamphenicol.and ciprofloxacin. Tetracyclins.

Psychoactive Drugs: Introduction, CNS depressants, CNS stimulants, sedatives and hypnotics, barbutirates. Synthesis of diazepam, phenytoins and glutethisimide.

Anti-neoplastic drug: Introduction; cancer chemotherapy, carcenoolytic antibiotic, plant derived anti-cancer agents (Taxol)role of alkylative agents and antimetabolites in treatment of cancer, mitotic inhibitors (elementary idea).

Cardiovascular Drugs: Introduction, cardiovascular diseases, synthesis of Amylnitrate. sorbitrate, quinidine, verapanil, methyl dopa and atenolol

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, Biotechonolgy and Clinical Chemistry of Enzmyes. Trevor Palmer (EWP)
5. Organic Chemistry by I.L.Finar Vol. II (ELBS Longamnn)
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. Chemsitry of Natural Products. S.V. Bhat, B.A. Nagasampagi, M. Siva Kumar. Naroosa Publishing House, New Delhi.

Course No: CH17407CR
Title: Advanced Quantum Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Electronic Structure Theory, Hartree-Fock Method (16 Contact hours)

Review: Electronic Hamiltonian, antisymmetrized wave function, Slater determinant. Hartree-Fock self-consistent field method. One and two-electron integrals in the light of minimal basis H_2 system.

Hartree-Fock Equation, Fock, Coulomb and exchange operators and integrals, restricted Hartree-Fock formalism, Roothaan equation. The Fock matrix elements, Koopman's theorem, Slater-Condon rules. Matrix form of Roothaan equation, the SCF procedure.

Basis Sets: Slatter-type orbitals, Gaussian basis sets. Model SCF calculations on H_2 /HeH^{+}.

Unit-II Configuration Interaction and Semiempirical methods (16 Contact hours)

Configuration Interaction: Electron correlation, configuration state functions, configuration interaction (CI), Brillouin theorem, full and truncated CI theories- CID, CISD, CISDTQ methods; Size consistency problem. Moller-Plesset and Coupled Cluster methods.

Semiempirical methods: The ZDO approximation; the PPP method, brief idea of CNDO, INDO and NDDO methods. The MINDO, MNDO, AM1 and PM3 methods.

Unit-III Density Functional Methods and Molecular Properties (16 Contact hours)

Density Functional Theory:Electron probability density. Hohenberg-Kohn theorems, Kohn-Sham formulation of DFT, n- and v- representabilities, E_x&$E_c$functionals; the local density and local spin density approximations, gradient corrected and hybridfunctionals.
Brief idea of Molecular mechanics methods, force fields.

Molecular Properties*:* Potential energy surfaces; molecular geometry and its optimization, Hessian Matrix and normal modes, vibrational frequencies, thermodynamic properties. Dipole moments, atomic Charges.

Unit-IV Use of Quantum Chemistry Software: Gaussian (16 Contact hours)

A quick tour of GAUSSIAN Interface. Input to Gaussian. Model calculations illustrating various features of the package**..**

1. A single point energy calculation: HCHO /CH3.CHO,HCHOMOs.
2. Geometry Optimization: Input and Output for ethene, fluoroethene, propene conformers
3. Transition state optimization $CH_2O \rightarrow HCOH$
4. NMR properties of ethane, ethene and ethyne.
5. Frequency Calculations: Input, Formaldehyde frequencies, Normal modes, zero point energy, thermodynamic properties, polarizability, hyperpolarazability.
6. Stationary points characterization –C3H5F
7. Model Chemistries: Basis set effect on HF bond length

8. Selecting an appropriate theoretical method:
    a) Electron correlation and post SCF methods, limitations of Hartree-Fock theory: HF bond energy, Optimization of O_3.
    b) Density Functional Theory: CO_2 structure and atomization energy.
    c) Butane / Isobutane isomerization energy, rotational barrier in n-butane.

9. Chemical reactions and reactivity:
    a) Hydration enthalpy of the reaction $H^+ + H_2O \rightarrow H_3O^+$
    b) Potential energy surfaces. Reaction path following (IRC calculation)
    $CH_2O \rightarrow HCOH$
    c) Heat of formation of CO_2 via an isodesmic reaction
10. Solvation models: Formaldehyde Frequencies in Acetonitrile

Books Recommended

1. Quantum Chemistry, Ira. N. Levine, (Prentice Hall, 2009).
2. Quantum Chemistry, 2nd Edn , D. A. McQuarrie, (University Science Books, 2007).
3. Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedmann, (Oxford, 2008).
4. Quantum Chemistry and spectroscopy, Engel & Reid, Pearson (2007)
5. Modern Quantum Chemistry - Introduction to Advanced electronic structure theory - A. Szabo & N. S. Ostlund, (Macmillan, 1982, Dover 1996).
6. Molecular Modeling, Principles and Applications, A. R. Leach, Prentice-Hall, 2001
7. Modern Electronic Structure Theory, D. R. Yarkouy (ed). (World Scientific, 1995)
8. Ab Initio Molecular Orbital Theory, by Hehre, Radom, Schleyer and Pople, (Wiley)
9. Density Functional Theory of Atoms and Molecules, R.G. Parr and W. Yang, Oxford(1989).
10. GAUSSIAN Manual, Gaussian Inc
11. Exploring chemistry with electronic structure methods, Foresman J.B., Frisch A., Gaussian Inc

Course No: CH17408CR
Title: Advanced Electrochemistry and Statistical Mechanics (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Instrumental Methods in Electrochemistry (16 Contact hours)

Fundamentals: Electrode potential and its measurement, standard and formal electrode potentials, three electrode measurements, uncompensated resistance.

Overview of electrode Processes: Faradaic and Non-Faradaic processes, factors affecting electrode reaction rate. Mass transfer: Convection, migration, diffusion, Fick's 1st and 2^{nd} law of diffusion,

Electrochemical Techniques:

Electrophoresis: Factors affecting ion migration, electro-osmosis, theory and applications of capillary electrophoresis.

Potential Step Methods: Chronoamperometry, Chronocoulometry at macro electrodes; theory and applications. Cottrell equation. Controlled-Potential coulometry, Constant-Current coulometric titrations.

Potential Sweep Methods: Linear sweep Voltammetry and Cyclic Voltammetry at macro electrodes theory and applications, Diagnostic criteria of Cyclic Voltammetry.

Unit-II Applied Electrochemistry (16Contacthours)

Electrochemistry of redox enzymes: Direct and mediated electron transfer, Enzyme modified electrodes-challenges and applications. Mechanism and approach to bioelectrosynthesis, examples of bioelectro synthesis-oxidation of alcohols, synthesis of dihydroxy acetone phosphate, site specific oxidation of sugars, reduction of carbonyl compounds, hydrogenation.

Energy storage devices: Desirable characteristics of energy storage devices, Discharge plot, Ragone plot. Batteries: Measures of battery performance. Classical batteries (Lead Acid, Nickel-Cadmium, Zinc-Mangenese dioxide). Modern batteries (Zinc-Air, Nickel-Metal Hydride, Lithium Ion Batteries), Supercapacitors.

Fuel cells, types of fuel Cells, basic fuel cell operation, kinetics of fuel cell reactions. Alkaline, Phosphoric acid, Polymer Electrolyte membrane and direct MeOH fuel cell, biofuel cells.

Unit-III Classical Statistical Mechanics and Ensemble concept (16 Contact hours)

Equations of Motion; Newton, Lagrange and Hamiltonian. Classical partition function, phase space and the Liouville equation, Kinetic theory of gases, equi-partition of energy, Maxwell's velocity distribution.

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. Statistical Mechanical treatment of imperfect gases. Virial equation of state from grand

partition function, virial coefficients in the classical limit, second and third virial coefficients.

Unit-IV Applied Statistical Mechanics (16 Contact hours)

Quantum Statistics: Fermi-Dirac and Boson-Einstein statistics, Nuclear spin statistics, symmetry and nuclear spin, Ortho and Para nuclear spin states, Ortho and Para Hydrogen and Deuterium, CO.

Application of grand partition function to Boson-Einstein and Fermi-Dirac statistics. Ideal Fermi-Dirac gas: Electrons in metals, Ideal Photon gas: Black body radiation, influence of wavelength for the Planck distribution, Bose-Einstein condensation.

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. Electrochemical Methods Fundamentals and Applications, 2ndEdition, Allen J.Bard, Larry R. Faulkner, John Wiley and Sons, INC.
2. Physical Electrochemistry-Principles, Methods and Applications, Israel Rubinstein (Ed.) Marcel Dekker, Inc. New York.
3. Understanding Voltammetry, 2nd Edition, Imperial College Press.
4. Elements of Molecular and Biomolecular Electrochemistry, Jean-Michel Saveant, Wiley-Interscience.
5. Electrochemistry, 2nd Edition, Carl H. Hamann, Andrew Hammett, Wolf Vielstich,Wiley-VCH.
6. Modern Electrochemistry 2B, 2nd Edition, J. O`M. Bockris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.
7. Statistical Thermodynamics, M. C.Gupta ,(NewAgeInternational,1993).
8. Statistical Thermodynamics-Fundamentals and Applications, N.M. Laurendeau, Cambridge University Press, 2005.
9. Statistical Mechanics, D.A. McQuarrie, (Viva,2003).
10. Introduction to Statistical Thermodynamics, Chandler, (OUP, 1987).
11. Statistical Thermodynamics and Kinetic Theory, C. E. Hecht, (Dover,1990).
12. Statistical Mechanics –Principles and Applications, Hill, Dover, 1987.
13. Statistical Thermodynamics for Chemists, A. Ben-Naim, (Plenum, 1992).
14. An introduction to Statistical Thermodynamics, Hill, (Addison-wesley,1987).

Course No: CH17409CR
Title: Chemistry of Materials (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Surfactant mixtures, Stimuli responsive surfactants and block copolymers (16 Contact hours)

Surfactant-Surfactant Interactions: Mixed micelle formation, mixed monolayer formation, synergism, Clint and Rubingh's models of mixed micelle formation**.** Importance and practical applications of mixed surfactant systems.

Stimuli-Responsive Surfactants: Introduction and applications: Biosurfactants, redox, photochromic, thermoreversible, pH-sensitive, cleavable and magnetic surfactants.

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

Unit-II Hydrogels and microemulsions (16 Contact hours)

Hydrogels: Introduction, Types of Hydrogels, Preparation, Properties and characterization of Hydrogels, Biomedical applications of Hydrogels.

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

Unit-III Langmuir Blodgett Films, Liquid crystals and Fullerenes (16 Contact hours)

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.

Fullerenes: Fullerenes- History, bonding, properties, doped fullerenes, fullerenes as superconductors and fullerene related compounds (carbon nanotubes).

Unit-IV Optical materials and Ionic conductors (16 Contact hours)

Optical materials: Luminesence and phosphors. Lasers – general principle of lasing action, Ruby laser, Neodymium-YAG lasers, semiconducing lasers and quantum dot lasers. Nonlinear optical effects, second and third order harmonic generation, nonlinear optical materials.

Ionic Conductors: Introduction to ionic conduction and mechanism. Types of ionic conductors, mechanism of ionic conduction, interstitial jumps (Frenkel); vacancy

mechanism. Super-ionic conductors: Diffusion and transition superionic conductors and mechanism of conduction in superionic conductors; examples and applications of ionic conductors.

Books Recommended:

1. M. J. Rosen, J. T. Kunjappu, “Surfactants and Interfacial Phenomena”, John Wiley & Sons, New York, 4^{th} Edition, 2012.
2. R. D. Vold and M. J. Vold, “Colloid and Interface Chemistry”, Addison-wesley, 1982.
3. .D. Y. Meyer, “Surfaces, Interfaces and Colloid”, VCH Publishers, Inc. 1991.
4. Jonsson, Lindmann, Homberg and Kronberg, “Surfactants and polymers in aqueous solution”, John Wiley and sons, 1998.
5. D. Fennell Evans, H. Wennerstrom, “The Colloidal Domain where physics, chemistry, biology and technology meet” VCH, New York, 1994.
6. Robert J. Hunter, “Foundations of Colloid Science”, Oxford University Press, New York, 2007.
7. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
8. I. W. Hamley, The Physics of Block Copolymers (Oxford University Press, Oxford, 1998.
9. N. Hadijichristidis, S. Pispas and G. A. Floudas Block Copolymers (Wiley, New York, 2003).
10. Introduction to Solids, Azaroff, Tata McGraw,1993.
11. SolidState Chemistry and its Applications, West, Wiley,1989.
12. The Physical Chemistry of Solids, Borg, Biens, Academic press, 1992.
13. Solid State Physics, N. W. Ashcroft and N. D. Mermin, Saunders college, 2001
14. Principles of Solid State, H. V. Keer, Wiley Eastern.
15. The Physics and Chemistry of materials, J.I. Gersten, F.W. Smith, John Wiley and sons, Inc. 2001.
16. Microemulsions: Background, New Concepts, Applications, Perspectives, C. Stubenrauch, Blackwell Publishing Ltd, 2009.
17. M. Sirousazar, M. Foroug, K. Farhad, Y. Shaabani and R. Molaei, Hydrogels: Properties, Preparation, Characterization and Biomedical, Applications in Tissue Engineering, Drug, Delivery and Wound Care, IN Advanced Healthcare Materials, Wiley online Library, 2014.

Course No: CH17410DCE

Title: Advanced Laboratory Course in Inorganic Chemistry (04 Credits)

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

External Exam: *75 Marks.* — ***Internal Assessment****: 25 Marks*

A: - Inorganic Preparations: (5 Experiments)

- Preparation of tetraamminecarbonatocobalt (III) nitrate and its conversion to pentaamminecholorocobalt (III) chloride.
- Preparation of trans dicholoro bis (ethylenediamine) cobalt (III) chloride and its conversion to cis-isomer.
- Preparation of tris (ethylenediamine) nickel (II) chloride dihydrate and its conversion to bis (ethylenediamine) nickel (II) chloride.
- Preparation of bis (acetylacetonato) copper (II) dihydrate.
- Preparation of pentaamminecholorocobalt (III) chloride and study of Linkage isomers by its conversion to pentaamminenitritocobalt (III) chloride and to nitro isomer followed by IR Characterization.

B:- Total analysis of a Coordination compound for determination of various components present.

(1- Experiment)

C: - Separation by Column Chromatography and Estimations: (5 Experiments)

- Separation of Permanganate and Bichromate ions on Alumina column and their Estimation from Beer Law plots.
- Determination of lonisable chloride in a Complex by cation exchange column (separation followed by Mohr's titration of elute for estimation).
- Separation of Cobalt (II) and Nickel (II) on anion exchange column followed by estimation through EDTA titrations.
- Separation of two Cobalt (III) complexes viz $[Co(NH_3)_6]Cl_3$ and $[Co(NH_3)_5Cl]Cl_2$ on Silica column.
- Ion exchange separation of Hydration / ionization isomers of Chromium (III) Chloride ($CrCl_3$).

D: - Potentiometric Titrations: (6 Experiments)

- Standardization of an Iron (ii) solution with a standard dichromate solution over Pt & Calomel assembly.
- Determination of purity of Ce (IV) Sulphate with a standard Iron (II) solution over Pt & Calomel assembly.
- Estimation of Iodide with Standard $AgNO_3$ over Pt & Calomel assembly using I^- \ I2 redox couple.
- Simultaneous determinations of Chloride and Iodide ions with Standard $AgNO_3$ over Ag-Glass electrode assembly.
- Determination of the purity of $[Co(NH_3)_5Cl]Cl_2$ over Ag-Glass electrode assembly.
- Complexometric titration for determination of Ferro cyanide with standard Zinc (ii) solution and inorder to establish the composition of the complex $K_2Zn_3[Fe(CN)_6]_2$

E: - pH-metric Titrations: (2 Experiments)

- Quantitative analysis of Chromate Dichromate mixture by pH Titration.
- Purity of Acetyl Salicylic acid (Asprin) in a commercial tablet by pH Titration.

F: - Conductometric Titrations: (2 Experiments)

- To determine the solubility and solubility product of a sparingly soluble salt ($BaSO_4$) in water.
- To determine the basicity of sodium potassium tartarate by Conductometric method.

G:- Spectrophotometry: (5 Experiments)

- Determination of Iron (II) with 1,10-Phenanthroline.
- Determination of Phosphate by Molybdenum blue method.
- Determination of formula of Iron (III) thiocyanate complex by Job's Continuous variation method.
- Determination of composition of Iron (II)—2,2-bipyridyl complex by Mole ratio method.
- Determination of rate of Aquation of complex $[Co(NH_3)_5Cl]Cl_2$ in acidic medium.

H: - Flame Photometry: (2 Experiments)

- Simultaneous determination of Sodium and Potassium in the given mixture.
- Determination of Cadmium and Magnesium in tap water.

Books Recommended:

- Vogel's quantitative analysis 6 Edn. Mendham, Denny; Pearson Education 2002
- Synthesis and Technique in Inorganic chemistry , G. S.Girlomi; R.J. Angleci 3rd edn.; University Science Books.
- Synthesis and characterization of Inorganic compounds W.AJolly
- Inorganic syntheses Vols II, VI Academic Press.
- Experimental Inorganic / Physical Chemistry ; Mounir A. Malati Horwood/1999.
- Quantitative Chemical Analysis ; 5th edn.; Harris ; Freeman ; 1999.
- Advanced Practical Inorganic Chemistry ; Adams ; Raynor, Wiley ; 1995.
- Advanced Experimental Inorganic Chemistry ; Ayodha Singh ; Campus Books 2002.

Course No: CH17411DCE
Title: Advanced Laboratory Course in Organic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *75 Marks.* ***Internal Assessment****: 25 Marks*

1. **Multistep synthesis of drugs/ organic coinpouiuls involving name reactions**
   (1) Synthesis oflocal 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.
2. **Extraction/Estimation of Organic compounds from Natural sources**
   (1) Isolation of lycopene and β-carotene from tomato and their characterization using *uv*- spectroscopy.
   (2) Isolation of limonene from its natural source and physicochemical analysis.
   (3) Assay of Belladona for Hyoscyamine.
   (4) Assay of lemon from citric acid and vitamin-C
   (5) Isolation of cholesterol from gallstone
   (6) Assay of coke (soft drink)
3. **Column Chromatography**
   Separation of two component solid mixture. Identification of separated components using physical, chemical and spectral techniques.
4. **Spcctrophotomctric estimation** (UV/visible)
   (1) Vitamin-C (Ascorbic acid)
   (2) Caffeine from tea.
   (3) Cholesterol
   (4) Aspirin
5. **Elcctrophoresis/ Paper chromatography**
   Separation and identification of aminoacids by elcctrophoresis / Paper chromatography.
6. **Spcctroscopy**
   Identification of Organic compounds through interpretation of their spectra (UV, IR, PMR, CMR and Mass. Spectra to be provided).

Books Recommended :

1. Comprehensive Practical Organic Chemistry, V.K. Ahluwalia, Renu Aggarwal (Univ. Press India Limited -2000).
2. Vogel's Text Book of Practical Organic Chemistry, B.S.Furniss, A. J. Hannaford (AWL 5th Ed.-1998).
3. Organic Laboratory Techniques , Donald .C. Pavia, Gary . M. Lampman (SCP 3rdEd.-1999)
4. Experiment Organic Chemistry, John.C. Gilbert., Stephen.F.Martin (SCP -1998)
5. Advanced Practical Organic Chemistry Vol. II, Jag Mohan (Himalaya Pub. House First Ed.-1992.

Course No: CH17412DCE
Title: Advanced Laboratory Course in Physical Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *75 Marks.* ***Internal Assessment****: 25 Marks*

A. Tensiometry
1. Investigation of variation of surface tension of n-butanol and sodium chloride solutions with concentration and hence determination of their surface excess concentrations using Gibb's Adsorption Isotherm.
2. Determination of CMC value of a detergent using tensiometry.

B. Cryoscopy
1. Investigation of variation of freezing point depression with concentration & determination of molecular mass.
2. Determination of the degree of dissociation of a salt/weak acid in solution.
3. Determination of activity co-efficient from freezing point measurements.

C. Spectrophotometry
1. To study the complexation reaction between Fe(III) & salicylic acid.
2. Determination of pK value of an indicator.

D. Spectrofluorometry
1. To determine the rate constant for fluorescence quenching of anthracene or perylene by CCl_4 in ethanol.
2. Using pyrene as probe determine the cmc of a surfactant and site of solubilization of pyrene in the micelle through spectrofluorometry.

E. Potentiometry
1. Precipitation titration of KCl, KBr, KI and their mixture with $AgNO_3$
2. Thermodynamics of a chemical reaction by EMF-method.
3. Determination of (a) Standard electrode potential & (b) Activity Coefficient.

F. Conductometry
1. Verification of Debye-Huckel-Onsagar law.
2. Precipitation titration of $BaCl_2$ and K_2SO_4/ $(NH_4)_2SO_4$
3. Estimation of the concentrations of H_2SO_4, CH_3COOH and $CuSO_4$ in a mixture.

G. Dynamic Electrochemistry
1. To estimate the surface area of a working electrode through chronoamperometry and chronocoulometry.
2. Using Cyclic Voltammetry to determine the formal potential and diffusion coefficient of $[Fe(CN)_6]^{3-}$.
3. Use cyclic voltammetry to determine the concentration of acetaminophen in a given sample.

H. Kinetics

1. Kinetic Investigation of BZ-Oscillatory reaction.
2. Kinetic study of enzyme catalyzed reaction (effect of pH and Temperature).

I. Viscometry and densitometery

1. Determination of Mol. Mass of a Polymer (Polyv inyl alcohol) using viscosity method.
2. To explore the nature of chemical bonding (head-head and Head tail linkage of monomers) in polyvinyl alcohol using Viscometry.
3. Determination of partial molar volume of sodium chloride solutions as a function of concentration from density measurements.

Books Recommended

1. Practical Physical Chemistry --- Findley revised by Kitchner.(Longman, 1971)
2. Experimental Physical Chemistry, A. M. Halpern, G. C. McBane, (Freeman, 2006)
3. Experiments in Physical Chemistry, 5th ed. --- Schoemaker et al. (MGH, 2003)
4. Experimental Electrochemistry---R. Holze (Wiley-VCH, 2009).

Course No: CH17413DCE

Title: Supramolecular Chemistry (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*

Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Supramolecular Interactions (08 Contact hours)

Definition and Development of Supramoleclar Chemistry. Nature of Supramolecular Interactions.

Hard Soft Acid Base Concept- Concept, Classification, Symbiosis. Utility in drug design and molecular recognition. Soft Ligands for Soft Metal Ions-Mixed Crown Ethers and Mixed Cryptands.

Unit-II Supramolecular Receptors (08 Contact hours)

Cation Receptors: Supramolecular Cation Coordination Chemistry, EDTA- The Supramolecular Host. Introductory account of Cation Receptors - Podands, Corands, Cryptands, Spherands and Calixarenes.

Anion Receptors: Scope and Challenges, Anion Hydrophobicity-Hofmeister Series, Introductory Account of Anion Receptors - Cyclophanes, Pyrolles, Azacrowns and Metal Based receptors. Hydride Sponge and Anticrowns.

Ion-Pair Receptors: Concept and Significance

Unit-III Crystal engineering and Supramolecular Motiffs (08 Contact hours)

Crystal Engineering: Introduction, Tectons and Synthons. Hydrogen Bond- Introduction, Criteria

Nature and Importance.

Self Assembly: Scope and Objectives. Concepts and Classification. Introductory Account of Coordination Capsules, Catenenes, Rotaxenes and Molecular Knots.

Unit-IV Network Solids and Molecular Devices (08 Contact hours)

Network Solids: Concepts and Classification, Network Topology. Zeolites: Structure, utility and limitations. Metal Organic Frameworks-Introduction and application in catalysis and Gas storage.

Molecular Devices**:** Philosophy of Molecular Devices, Photophysical Fundamentals and Mechanism of Energy and Electron Transfer, Introductory Account of Molecular Wires, Molecular Switches and Molecular Motors.

Books 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, Ist 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. Chemical Reviews. Vol. 115, Issue 15, year **2015**, Pages 6999-8156
8. Introduction: Supramolecular Chemistry. F. Huang and E. V. Anslyn. Chem. Rev. **2015**, 115, 6999−7000.
9. Supramolecular materials. D. B. Amabilino, D. K. Smith and J. W. Steed. Chem. Soc. Rev., **2017**, 46, 2404—2420
10. A Bond by Other Name. G. R. Desiraju. Angew. Chem. Int. Ed. **2011**, 50, 52-59.
11. The Weak Hydrogen Bond: In Structural Chemistry and Biology. G. Desiraju, T. Steiner. **Oxford, IUCr Monograph on Crystallography**.

Course No: CH17414DCE
Title: Designing Organic Synthesis (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I (A) Oxidative and Reductive Processes in Organic Synthesis (8 Contact hours)

Oxidation**:** Introduction, Aromatisation of cycloalkanes and alkenes using metal catalysts and DDQ. Oxidation of Alcohols using chromic acid, DCC and Swern reagent. Oppenaur oxidation. Oxidation of ketones. Oxidation at activated carbon-hydrogen bond. Oxidation with Selenium dioxide. Prevost hydroxylation and its modification by Woodward.

Reduction**:** lntroduction. Reduction of Alkenes, Alkynes and Aromatic rings.

Reduction of carbonyl compounds: Clemmensen and Wolf-Kishner reductions. Reductions using $LiAlH_4$ and $NaBH_4$ Bouveault-Blanc reduction. Reduction of Epoxides, Nitro, Nitroso, Azo and Oxime groups. Reductions using Tributyl Tin Hydride.

(B) Protection and Interconversion of Functional Groups (8 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-II 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, α, β-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; Verlage VCH;1986.
3. Principles of Organic Synthesis 2nd edn;. R. O. C. Norman; Chapman and Hall; 1978.
4. Advanced Organic Chemistry Part B, 5th edn.; F. A. Carey and R.J Sundberg ; Springer; 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, 6lh Ed., J. March,; Wiley; 2012.
9. Organic Synthesis- The disconnection Approach; Sturat Warren; Wiley; 2013

Course No: CH17415DCE
Title: Computational Chemistry (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I

(a) Numerical solution of equations (8 Contact hours)

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

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

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

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

(b) Numerical differentiation and integration (8 Contact hours)

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

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

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

Unit-II

(a) Interpolation and Curve Fitting (8 Contact hours)

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

Lagrange’s interpolation method, Newton’s divided differences, Cubic spline, piece wise interpolation.

Least squares approximation, linear and quadratic.

(b) Use of Mathematica/Scilab for numerical solution of problems(8 Contact hours)

The mathematica package will be used for the solution of problems covered under the above three units.

Books Recommended

1. Data Reduction & Error Analysis, Bevington& Robinson, (McGraw-Hill, 2003)
2. Computational Chemistry, A. C. Norris, (Wiley.)
3. Computer Software Applications in Chemistry - P. C. Jurs, (John Wiley, 1996.)
4. Numerical Methods for Scientists and Engineers, H. M. Antie, (TMH,).
5. Numerical Recipes in Fortran/C, W.H. Press et al., (CUP,1992)
6. Applied Numerical Analysis, Gerald &Wheatly, (Pearson Education, 2002)
7. Mathematical Methods for Scientists and Engineers, D.A. McQuarie, Viva Books, 1st Ed., 2009.
8. Mathematica Manual.

Course No: CH17416DCE
Title: Seminar (02 Credits)

Presentation by a candidate on any topic chosen in consultation with the teacher incharge.

(25 Marks)

Manuscript (on the topic) submission (25 Marks)

Course No: CH17417GE
Title: Synthetic Polymers and their Applications (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

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

Course No: CH17418GE
Title: Novel Materials (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

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

Block Copolymers: Introduction: classification, micellization of diblock 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, photoconductivity and sensors.

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

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

Luminesence and phosphors. Lasers - general principle of lasing action, Ruby laser, semiconducing 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 Nanofluids 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, Jeremy Ramsden and Ventus Publishing ApS, 2009.

Course No: CH17419OE
Title: Food Chemistry (02 Credits)

Max. Marks: *50* — ***Duration:*** *32 Contact hours*

Ist Unit Exam: *25 marks* — ***IInd Unit (Term end) Exam:*** *25 marks*

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_2, 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; 3rd Ed.; Marcel Dekker, Inc. NY; 2005.
2. Food: The Chemistry of its components; T.P. Coultate; 3rd 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; 2nd ed.; Springer International Edition; 2005.

Course No: CH17101CR
Title: Inorganic Chemistry (04 Credits)

Max. Marks: *100* — ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Stereochemistry and Bonding in the Compounds of Main Group Elements (16 Contact hours)

Valence bond theory: Energy changes taking place during the formation of diatomic molecules; factors affecting the combined wave function. Bent's rule and energetics of hybridization.

Resonance: Conditions, resonance energy and examples of some inorganic molecules/ions.

Odd Electron Bonds: Types, properties and molecular orbital treatment.

VSEPR: Recapitulation of assumptions, shapes of trigonal bypyramidal, octahedral and pentagonal bipyramidal molecules / ions. (PCl_5, VO_3^-, SF_6, $[SiF_6]^{2-}$, $[PbCl_6]^{2-}$ and IF_7). Limitations of VSEPR theory.

Molecular orbital theory: Salient features, variation of electron density with internuclear distance. Relative order of energy levels and molecular orbital diagrams of some heterodiatomic molecules /ions. Molecular orbital diagram of polyatomic molecules / ions.

Delocalized Molecular Orbitals: Butadiene, cyclopentadiene and benzene.

Detection of Hydrogen Bond: UV-VIS, IR and X-ray. Importance of hydrogen bonding.

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

Stepwise and overall formation constants. Inert & labile complexes. Stability of uncommon oxidation states.

Metal Chelates: Characteristics, Chelate effect and the factors affecting stability of metal chelates.

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-III Bonding 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 ML6; Effect of pi-bonding. Molecular orbital and energy level diagram for bonding in Ferrocene, Square-planar and Tetrahedral complexes.

Unit-IV Pi-acid Metal Complexes **(16 Contact hours)**

Transition Metal Carbonyls: Carbon monoxide as ligand, synthesis, reactions, structures and bonding of mono- and poly-nuclear carbonyls. Vibrational spectra of metal carbonyls for structural diagnosis.

Prepration, reactions, structure and bonding of transition metal nitrosyls, dinitrogen and dioxygen complexes.

Tertiary phosphine as ligand.

Books Recommended

1. Principles of Inorganic Chemistry; 1st edn.; Brain W. Pfennig; Wiley; 2015.
2. Advanced Inorganic Chemistry; 5th. and 6th edn; F.A. Cotton , G. Wilkinson; Wiley; 1998/1999.
3. Inorganic Chemistry; 4th edn; J. E. Huheey; E. A. Keiter; Harper Collins; 2009.
4. Inorganic Chemistry; G. Wulfsberg; Viva; 2002.
5. Chemistry of the Elements; 2nd edn; N. N. Greenwood, A. Earnshaw; Butterworth; 1997.
6. Inorganic Chemistry; 3rd edn; D. F. Shriver; P. W. Atkins; Oxford; 1999.
7. Inorganic Chemistry; K.F. Purcell, J.C Kotz; Saunders; 1977.
8. Coordination Chemistry; D. Banerjea; Tata McGraw Hill; 1993.

Course No: CH17102CR
Title: Organic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Delocalized Chemical bonding (16 Contact hours)

Overview: Inductive effect. Conjugation, Cross conjugation, Hyperconjugation–Isovalent and sacrificial hyperconjugations, Acids / Bases, Nucleophiles and Electrophiles. Resonance, Rules for writing resonance structures, Steric inhibition of resonance.

Tautomerism: Different types including valence 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.

Unit-II Reactive Intermediates and Determination of Reaction Mechanism (16 Contact hours)

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

Determination of Reaction Mechanism: Reaction Mechanism & Types of reactions. Determining reaction mechanism: Structure of Product, Transition states & Intermediates (Hammond postulate). Catalysis including acid and base catalysis, Specific acid and base catalysis. Fate of individual atoms (Isotope Labeling). Stereochemical course of reaction. Thermodynamic and kinetic evidences. Correlation of structure – reactivity.

Unit-III Stereochemistry: (16 Contact hours)

Chirality: Introduction, Chirality due to chiral centre. Molecules with more than one Chiral centres, Threo and erythro isomers. Convention for of assigning D, L & R, S configurations. Optical activity due to chiral axis, chiral plane and helicity. Chirality involving atoms other than carbon. Chirality in metallic complexes. Enantiotopic and diastereotopic atoms, groups and faces.

Asymmetric Synthesis: Introduction and principle of asymmetric synthesism. Principal categories of asymmetric synthesis. Use of chiral substrates. Diastero-selectivity in Aldol reactions. Sterospecificity and steroselectivity of enzymes.

Confirmations: Origin of conformational energy. Angle and Pitzer strain. Conformational analysis of cycloalkanes, and decalines. Effect of conformation on reactivity in acyclic and cyclic systems. Conformation of sugars & anomeric effect. Conformation of cyclohexene, cyclohexanones and bicycloheptane – a bridged system.

Unit-IV Aliphatic Nucleophilic Substitutions : (16 Contact hours)

Mechanism and stereochemical implications of S_N2, S_N1, S_Ni and Neighbouring Group Participation (by π and σ-bonds) reactions. Comparison of S_N1 and S_N2 reactions. Effect of substrate structure, attacking nucleophile, leaving group and solvent on the rates of S_N1 and S_N2 reactions. Mixed S_N1 and S_N2 reactions. Nucleophilic substitution at allylic, benzylic, aliphatic trigonal and vinylic carbons. Nucleophilic substitution in alcohols, Mitsunobu reactions. Nucleophilic substitutions on other elements. Functional group transformation using S_N2 reactions in organic synthesis. Nucleophilic substitutions in biological systems.

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

Aliphatic Electrophilic Substitutions: General mechanism of S_E1, S_E2 and S_Ei reactions. Mechanisms of reactions involving migration of double bond. Effect of substrate, leaving group and solvent on reactivity. Stork-Enamine reaction.

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 3rd Ed., S.M. Mukherjee and S.P. Singh. (Macmillan-1998).
4. Stereochemistry of Organic Compounds 2nd Ed., D. Nasipuri. (New Age Inter.- 2008)
5. Stereochemistry of Carbon Compounds - E.L.Eliel. (TMH -2007)
6. Stereochemistry of Organic Compounds 7th Ed. - P.S. Kalsi. (New Age Inter.- 2012).
7. Organic Chemistry - 2nd Ed., J. Hornback. (Brooks/Cole- 2006,
8. Organic Chemistry, 5th Ed., John McMurry. (Brooks/Cole-2000).
9. Advanced Organic Chemistry, 5th Ed., F.A Carey & R.J Sundberg (Springer-2007).
10. Organic Chemistry, 2nd Ed., Jonathan Clayden (OUP-2012)
11. Organic Chemistry, 11th Ed., Solomons, T.W.G., (Wiley-2015).

Course No: CH17103CR
Title: Physical Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

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)

Theories of Chemical Reactions: Activated complex theory of reaction rates, statistical & thermodynamic formulations, comparison with collision theory. Theories of unimolecular reactions (Lindman, Hinshelwood , RRK and RRKM theories), Introduction to potential energy surfaces.

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

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

Unit-IV Chemical kinetics-II **(16 Contact hours)**

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

Reactions in solutions: Diffusion controlled reactions (partial & full microscopic diffusion control), Ionic Reactions; Single & double sphere models of ionic reactions.

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

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

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. CH17104DCE
Title: Laboratory Course in Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *75 Marks.* ***Internal Assessment****: 25 Marks*

I. Preparation of Coordination compounds of Transition metals:

1. Theoretical appraise of first row Transition metal Coordination Chemistry.
2. Synthesis as a Laboratory Technique (Concepts, Calculations and Design of Synthetic procedures).
3. Selected preparations of the following coordination compounds with the specific objectives:

i) Mercurytetrathiocyanatocobaltate(II)	:	To visualize the complexation process.
ii) Tristhioureacopper(I)sulphate monohydrate	:	Insitu generation and Stabilization of unusual oxidation state and re-crystallization /crystal growing
iii) Hexaamminecobalt(III) chloride	:	Multistep synthetic procedure
iv) Trisethylenediaminecobalt(III) chloride	:	Two stage synthesis and aerial oxidation/Resolution of a racemic mixture
v) Ammonium dodeca molbedophosphate	:	Synthesis of a heteroploy metallate/ Bonding and structure.

II. 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.

III.

A. Qualitative Analysis by Semi micro Technique:

Discussion about the analysis scheme. Analytical groups and Group reagents. Scales of Analysis, Skill of semi micro technique. Chemistry involved in separation and identification of less familiar cations by semi micro analysis.

B. Identification of four less familiar cations from different analytical groups with simple and complex combinations:

(i) Group I and II A
(ii) Group I, II A and II B
(iii) Group IIA and II B
(iv) Group I and Group III
(v) Group II B and Group III
(vi) Group III only.

IV. Inorganic Quantitative Analyses:

A. **Gravimetry:**

i) Skill and importance of weighing in Chemistry, Gravimetreric 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.

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) Barium (Ba^{2+}) as BaSO4 and Zinc as $[ZnEDTA]^{2-}$ complex.

iii) Barium (Ba^{2+}) as $BaSO_4$ and Nickel (Ni^{2+}) as $[NiEDTA]^{2-}$ complex.

iv) Nickel (Ni^{2+}) as Ni $(dmg)_2$ complex and Magnesium (Mg^{2+}) as $[Mg\ EDTA]^{2-}$ complex.

v) Copper (Cu^{2+}) as CuSCN and Magnesium (Mg^{2+}) as $[MgEDTA]^{2-}$ complex.

Books Recommended:

1. Advanced Inorganic Chemistry, 5th ed. / 6th 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; 5th edn; Jeffery, Bassett; (ELBS, 1989).
4. Quantitative Analysis; 6th edn; Day, Underwood (Printice Hall, 1993).
5. Analytical Chemistry, 6th Ed; D. Christian, Wiley.
6. Quantitative Analysis; 6th edn; Day, Underwood (Printice Hall, 1993).

Course No: CH17105DCE
Title: Symmetry and Group Theory (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

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, Symmetry groups and group multiplication tables.

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 Orthoganality Theorm-elementary idea, consequences of the Great Orthogonolity Theorem. Reducible and Irreducible representations, Mullikan symbols for IRS. Character table-construction of character tables for C2v, C3v and C4v point groups.

Applications of group theory to IR and Raman spectroscopy, 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 and Polarity.

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.

Course No: CH17106DCE
Title: Infrared, Raman and Electronic Spectroscopy (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

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_2, O_2),

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. Physical Methods for Chemists; R.S.Drago; 2nd edn; Saunders; 1992.
2. Fundamentals of Molecular Spectrsocopy; C.N.Banwell, E.M.Mc Cash; 4th edn; Tata McGrawHill; 1994.
3. Physical chemistry; P. W. Atkins; 6th edition; Oxford University Press; 1998.
4. Electronic Absorption Spectroscopy and related techniques; D N Sathyanarayna; UniversitiesPress.
5. Introductory Raman Spectroscopy; J. R. Ferraro, K. Nakamoto & C. W Brown; 2nd edn; Academic Press 2005.
6. Theory and Applications of Ultraviolet Spectroscopy; H.H.Jaffe, M.Orchin; Wiley; 1962.
7. Molecular Spectroscopy; 1st edn; J L. McHale; Prentice Hall; 1999.
8. Modern Spectroscopy; J.M.Hollas; Wiley; 1987.
9. Basic Principles of Spectroscopy; R.Chang; McGraw Hill; 1971.
10. Structural Methods in Inorganic Chemistry; 2nd edn; E.A.V.Ebsworth, D.W.H.Rankin, S.Cradock; Blackwell; 1991.

Course No: CH17001GE
Title: Chemistry of the Environment (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Soil and Hydrosphere (16 Contact hours)

Soil: Nature and Composition of soil – Air, Water, Inorganic components, organic matter and humus. Acid – Base and Ion exchange reactions in soil.

Wastes and pollutants in soil: Chemical degradation, photochemical reactions and biodegradation. Desertification, Deforestation and soil erosion.

Hydrosphere: Chemical Composition of Water Bodies: Lakes & rivers, Factors determining composition (thermal stratification, acid-base, pE concept).

Aquatic pollution: Inorganic, Organic, Pesticide, Agricultural, Industrial and Sewage.

Water quality parameters: Dissolved oxygen, Metals, Content of Chloride, Phosphate, Nitrate, and Microorganisms. Water quality standards.

Analytical Methods for determining BOD, DO, COD, and choice of methods for determining metals (As, Cd, Hg, Pb & Se).

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

Unit-II Atmosphere (16 Contact hours)

Chemical Composition of the Atmosphere: Particles, ions, radicals and their formation. Vertical profile of the atmosphere, Heat budget of earth's atmospheric system. Chemical and photochemical reactions in atmosphere, photochemical smog formation.

Oxides of N, C, S and their effects.

Ozone layer: Formation of ozone and mechanism of ozone depletion.

Pollution by chemicals: Chlorofluorocarbons, hydrocarbons and ozone.

Green house effect: Cause, source and impact on global climate.

Consequences of Green house effect and remedial measures.

Acid rain: Chemical aspects, adverse effects and control.

Books Recommended

1. Environmental Chemistry; 5th edn; Colin Baird; Freeman & Co; 2012.
2. Environmental Chemistry; 9th edn.S.E.Manahan; Lewis Publishers;2009
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 pollution; B.K.Sharma & H.Kaur; Goel Publishcrs;1996.
7. Environmental Chemistry; Nigel. J.Bunce; Wurez Publishers; 1991.
8. Environmental Toxicology; Ed.Rose; Gordon & Breach Science Publishers.

Course No: CH17002GE
Title: Surfactants and their Applications (02 Credits)

Max. Marks: *50*	***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks*	***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Self-Assembly of Surfactants (16 Contact hours)

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 Systems (16 Contact hours)

a) **Mixed Surfactant systems**: Mixed micelle formation, mixed monolayer formation, synergism, various models of mixed micelle formation(Clint, Rubingh, Motamurra, Blankschtein, and Rubing-Holland models) 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. Characterization of polymer- surfactant systems by various techniques like viscosity, light scattering, spectroscopic and conductance measurements. 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. Physical Chemistry; P.W. Atkins; ELBS; Oxford; 1994.
3. Principles of Colloid and Surface Chemistry; P.C. Heimenz; Marcel Dekker Inc; New York; 1986.
4. Surfactants and Interfacial Phenomena; M. J. Rosen; John Wiley & Sons; New York; 1989.
5. Colloid and Interface Chemistry; R. D. Vold and M. J. Vold; Addison-Wesley; 1982.
6. Surfaces, Interfaces and Colloid; D. Y. Meyer; VCH Publishers; Inc; 1991.
7. Surfactants and polymers in aqueous solution; Jonsson, Lindmann, Homberg and Kronberg; John Wiley and sons; 1998.
8. Advances in Colloid and Polymer Science; B.K.Paul & S.P.Moulik, Current Science,Vol.80,p 990-,2001; Vol.78,p 99,1998.
9. Critical Reviews in Food Science and Nutrition; John Flanagan & Harjinder Singh, ,Vol. 46, pp221-237, 2006.
10. Advanced Drug Delivery Reviews; M. J. Lawrence & G.D.Rees; Vol, 45, p 898, 2000.
11. Energy Fuels; T. N. Dantas, A.A.D, Netoetal; DOI:10.1021/ ef900952y; 2010.

Course No: CH17001OE
Title: Chemistry in Everyday Life   (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*

Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

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

(a) Water- An Amazing Chemical Stuff

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)

Course No: CH17201CR
Title: Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

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

Energy profile of a reaction; reactivity of metal complexes; inert and labile complexes.
Types of substitution reactions; mechanistic classification of substitution reactions:- Dissociative, Associative, Dissociative conjugate base and Interchange.
Empirical criteria to differentiate the mechanism of substitution reaction.
Substitution in octahedral complexes- Classification of metal ions based on water exchange rates. Metal-complex formation- the Eigen-Wilkins mechanism. Anation reactions.
Hydrolysis Reactions; Simple Acid hydrolysis, Acid catalysed and Base hydrolysis. Stereochemical changes in Octahedral Substitution Reactions.
Substitution reactions without breaking of metal-ligand bond.

Unit-III Mechanism of Ligand Substitution Reactions in Square-Planar complexes: (16 Contact hours)

Significance of the two-term rate^law, Mechanism, and Steric course of the substitution reactions.
Factors affecting the rate of substitution:- entering and leaving groups; nucleophilicity of entering group and the n_{pt} scale, central metal ion, solvent and the non-leaving groups.
The Trans effect;- Theories, applications in synthesis.
cis-trans isomerization in square planar complexes.

Unit-IV Organo Metallic Compounds (16 Contact hours)

Introduction, Nomenclature, classification and importance of organometallic compounds.

Nomenclature and Classification of Organometallic compounds.

Effective atomic number (18-Valance electron) rule and its significance.

Stability of Organometallic Compounds towards heat, oxidation and hydrolysis.

Preparation, Properties, Structure, bonding and applications of Alkyls and aryls of Li, B and Al.

Synthesis, Structure and bonding in Zeise's Salt.

Homogenous Catalysis using Organometallic Compounds: Catalysis, Terminology of Catalysis and Tolman Catalytic loop;

Oxidative addition, reductive elimination and migration (insertion) reactions.

Hydrogenation and Hydroformation reactions in alkenes.

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. CH17202CR
Title: Organic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Aromatic Electrophilic Substitution (16 Contact hours)

Overview: Arenium ion mechanism, Sigma and pi – complexes, Energy profile diagram, Effect of leaving group. Orientation and reactivity in mono substituted benzene ring , *Ortho / Para ratio*, Ipso attack.

The Third substitution : Orientation of substitution in benzene ring with more than one substituent. Orientation in other ring systems. Carboxylation of aromatic rings with $COCl_2$ and amidation with NH_2COCl. Reversal of F.C. acylations. 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 mechanism (S_N1, S_NAr, Benzyne and $S_{RN}1$). Structure reactivity relationships. Effect of leaving group and attacking nucleophile. Mechanisms of Von-Richter, Sommelet-Hauser and Smiles rearrangements and Chichibabin reaction.

Free Radical Substitution:

Free radical substitution mechanisms. Mechanisms at an aromatic substrate. Neighbouring Group Assistance in free radical reactions, Reactivity for aliphatic and aromatic substrates. Reactivity in the attacking radical. Effect of solvent on reactivity.

Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sandmeyer reaction, free radical rearrangements and Hunsdiecker reaction.

Unit-II Addition to multiple bonds. (16 Contact hours)

Addition to carbon-oxygen double bonds:

Overview of reactivity carbonyl compounds: Mechanisms of addition of water , hydrogen cyanide, alcohols , amines , organometallic reagents and hydrides to aldehydes and ketones.

Mechanism of Wittig, Mannich , Aldol, Cross Aldol , Cannizarro's , Knoevenagel, Robinson annulation, Claisen, Dickman , Benzoin , Perkin and Stobbes reactions.

Addition to carbon-carbon multiple bonds:

General mechanism, reactivity, orientation and stereochemical implications of additions reactions involving electrophiles, nucleophiles and free radicals. Addition to cyclopropane ring. Hydrogenation of double/triple bonds and aromatic rings. Hydroboration, Ene-reaction, Michael reaction and Sharpless assymetric epoxidation.

Unit-III Molecular Rearrangements (16 Contact hours)

General mechanistic treatment of nucleophilic, electrophilic and free radical rearrangments. Nature of migration and migratory aptitude and memory effect. Detailed study of following rearrangements: Wagner-Meerwein, Pinacol- Pinacolone, Demyanov, Benzil-Benzilic acid, Favorskii, Arndt-Eistert, Neber, Hofmann, Curtius, Lossen, Schmidt, Beckmann, Baeyer-Villiger, Pyne and Dienone - phenol rearrangements.

Unit-IV Pericyclic reactions. (16 Contact hours)

Molecular orbital symmetry, Frontier orbitals of ethene, 1,3- butadiene, 1,3,5-hexatriene and allylic systems. HOMO, LUMO concept, FMO approach. Classification of Pericyclic reactions. Woodward Hofmann rules for the following pericyclic reactions. Cycloadditions: Thermal and Photochemical 2+2 and 4+2 cycloadditions. Suprafacial and antrafacial cycloadditions.

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

Sigmatropic rearrangements: Classification, [1,3], [1,5] and [3,3] sigmatropic shifts. Cope and Claisen rearrangements. Suprafacial and antrafacial shifts of hydrogen atom.

Books Recommended

1. Advanced Organic Chemistry Reactions, Mechanism and Structure, 4th Ed.,Jerry March. (Wiley, 1999).
2. Advanced Organic Chemistry 4th Ed. - F. A. Carey and R. J. Sundberg. (Plenum, 2001).
3. A Guide Book to Mechanism in Organic Chemistry 6th Ed.- Peter Sykes. (Longman, 1996).
4. Structure and Mechanism in Organic Chemistry 2nd Ed. - C. K. Ingold. (CBS, 1994).
5. Modern Organic Reactions 2nd Ed. - H.O. House (Benjamin, 1972)
6. Principles of Organic Synthesis 2nd Ed. - R.O.C. Norman (Chapmann Hall, 1978)
7. Reaction Mechanism in Organic Chemistry 3rd Ed. - S.M. Mykherjee and S.P. Singh. Macmillan, 1998).
8. Organic Chemistry - J. Hornback,pk. (Brooks/Cole, 1998).
9. Fundamentals of Organic Cbemjstry , 5th ed.- Solomons. (Wiley, 1992).
10. Organic Chemistry, 5th Ed.- John McMurry. (Brooks/Cole, 2000).

Course No: CH17203CR
Title: Physical Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I 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.

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.

Ion solvent Interactions*:* Non structural (Born) treatment and an introduction to structural (Ion-dipole, Ion-quadruple) 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.

Unit-III Biophysical Chemistry (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 (synthesis & hydrolysis), Principles of coupled reactions and their importance for living systems.

Biopolymers: Molecular forces and Chemical bonding in Bio-polymers, hydrophobic interactions, structure of proteins, protein folding and unfolding. Biological membranes, phase transitions in biological membranes. Donan effect and transport across biological membranes.

Binding of Ligands and metal Ions to bio-macromolecules, one binding site per macromolecule, n equivalent binding sites per macromolecule, binding of oxygen to myoglobin and hemoglobin.

Unit-IV Statistical Thermodynamics (16 Contact hours)

Concept of distribution, thermodynamic probability and most probable distribution. Sterling approximation. Method of undetermined multipliers.

Distribution Laws: Derivation of Boltzmann distribution law, Bose-Einstein and Fermi-Dirac laws (without derivation) and their comparison with Boltzmann distribution law.

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

Books Recommended:

1. Physical Chemistry –P. W. Atkins, 9th Edition, 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, Lioyd L Lee, World Scientific, 2008.
7. An Introduction to Aqueous Electrolyte Solutions, Margaret Robson Wright, Wiley, 2007.
8. Modern Electrochemistry 1, 2A, 2nd Edition, J. O`M. Bokris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.
9. Physical Chemistry for the Biosciences, Raymond Chang, University Science Books, 2005.
10. Physical Chemistry for the Life Sciences,2nd Edition, Peter Atkins, Julio de Paula, Oxford University Press2015.
11. Statistical Thermodynamics, M.C.Gupta, New Age International, 1993.
12. Statistical Mechanics, Agarwal, Eisner, Wiley, 1991.

Course No: CH17204DCE

Title: Laboratory Course in Organic Chemistry (04 Credits)

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

***External Exam:** 80 Marks.* — ***Internal Assessment**: 20 Marks*

1. **Qualitative Analyses of Organic Compounds**

   (i) **Physical Properties:** Physical state, colour, odour, solubility behavior 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, Nitrocompounds and Hydrocarbons.

   (iii) **Preparation and recrystallization of the derivatives of above mentioned group of compounds.**

2. **Separation, Purification and identification of Organic compounds from a three component mixture:**

   (a) **Separation based on solubility in water and organic solvents.**

   (b) **Separation based on Chemical properties:** Solubility in Sodium bicarbonate, Sodium Hydroxide and Hydrochloric acid.

   (c) **Identification of individual components using physico-chemical properties**

3. **Detection of functional groups using IR spectroscopy (spectra to be provided)**

4. **Quantitative Estimation of the following compounds**

   (a) Glucose.

   (b) Glycine

   (c) Acetone

   (d) Phenol.

   (e) Ascorbic acid.

5. Organic Preparations

(a) Acetylation of Cholesterol or salicylic acid.

(b) Oxidation of Cyclohexanol by chromic acid to get adipic acid.

(c) Aldol condensation: Dibenzal acetone and benzaldehyde.

(d) Cannizarro's reaction of 4-Chlorobenzaldelyde.

(e) Aromatic electrophillic substitutions in benzene, benzoic acid or aniline.

(f) Beckman rearrangement starting from acetophenone.

(g) Haloform reaction: Preparation of Iodoform.

Books Recommended:

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

Course No: CH17205DCE
Title: NMR and ESR Spectroscopy (02 Credits)

Max. Marks: *50* — ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I NMR Spectroscopy-I (08 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 (T1, T2). Shielding and deshielding of magnetic nuclei. Chemical shift, its measurement and factors influencing chemical shifts; local paramagnetic and diamagnetic shielding, neighboring group anisotropy and ring currents in aromatic systems

Unit-II NMR Spectroscopy-II (08 Contact hours)

Spin- Spin coupling, coupling constants. Examples.
Vicinal coupling and electron correlation. Chemical equivalence and magnetic equivalence.
Fermi contact and Dirac Vector Model. Effect of Chemical exchange on spectra.
Double resonance techniques; spin decoupling, nuclear overhauser enhancement.
Instrumentation; FT-NMR and its advantages. NMR studies of nuclei other than proton – ^{13}C, ^{19}F and ^{31}P.

Unit-III ESR spectroscopy-I (08 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

Unit-IV ESR spectroscopy-II (08 Contact hours)

Fermi contact, Spin polarization effects, Dipolar coupling, Mc Conell equation and calculation of spin densities in inorganic radicals such as $CO_2^{-\bullet}$, $CH_3^{\bullet}$, $BH_3^{-\bullet}$ and $F_2^{-\bullet}$.
Spin orbit coupling and significance of g tensors.
Zero field splitting and Kramer's degeneracy (fine structure),
Advance Applications

Books Recommended

1. Introduction to Spectroscopy; 3rd edn.; D. L. Pavia, G. M. Lampman, G. S. Kriz; Saunders-Thomson learning; 2001.
2. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry; R. V. Parish; Ellis Horwood; 1990.
3. Nuclear Magnetic Resonance; P. J. Hore; Oxford; 1995.
4. Principles of Instrumental Analysis; 4th edn.; D. A. Skoog, J. J. Leary; Saunders; 1992.
5. Physical Methods for Chemists; 2nd edn.; R. S. Drago; Saunders; 1992.
6. Basic Principles of Spectroscopy; R. Chang; McGraw Hill; 1971.
7. Introduction to Magnetic Resonance; A Carrington, A. D. McLachlan; Harper & Row; 1967.
8. NMR and Chemistry; 2nd edn.; J. W. Akitt; Chapman and Hall; 1983.

Course No: CH17206DCE
Title: Solid State Chemistry (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Structure and Theories of Solids (16 Contact hours)

Structure of solids: 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. *S*tructure 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, Colour centres, Dislocations and their types.

Theories of solids:

Free electron theory of metals**:** The Drude Model, Lorentz modification, Sommerfield Model; Fermi-Dirac distribution function, Density of states, electronic heat capacity, Hall effect.

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. 10^{th}, 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: CH17207GE
Title: Metal Ions in Living Systems (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Alkali and Alkaline Earth Metal-ions in Biosystems (16 Contact hours)

Biomolecules and their Metal Coordination behavior.

Evidence of the presence of metal ions in biological systems (Direct / Indirect). Classification of metals and non-metals according to their action in biological systems.

Essential Elements: Concept of essentiality, criteria and classification of essential elements as per their role in living systems.

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.

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. Dioxygen transport (Haemocyanin).

Zinc in Biosystems: Lewis acid catalyst, Enzyme activator in vitamin B_{12}.

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

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

Antibacterial, Antiviral and Antifungal activities of metal complexes: Labile and Robust metal complexes; probable mechanism of action.

Books Recommended

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

Course No: CH17208GE
Title: Bio-Physical Chemistry (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Bioenergetics & Equilibrium in biological Systems (16 Contact hours)

Relevence of thermodynamics to Biological systems, Biochemists standard state, standard energy changes in biochemical reactions, ATP as energy currency of cell (synthesis & hydrolysis). Principles of coupled reactions and their importance for living systems.

Acid–base Equilibria: pH, pKa & pKb values. Dissociation of Amino-acids, isoelectric point. Buffer solutions, buffer capacity, effect of ionic strength & temperature, maintaining pH of blood.

Electrochemical equilibria: Standard redox potential, half- cell potentials of biological reactions, Nernst Equation.

Biological Membranes, Transport of ions across biological membranes, active and passive transport. Theory of membrane potential.

Unit-II Bio-electrochemistry, Kinetics & Spectroscopy (16 Contact hours)

Electrochemistry of Nerve conduction, medical applications of electrochemistry.

Renaturation of DNA as a second order reaction, Enzyme kinetics, Michaelis-Menton mechanism, competition & inhibition, multisubstrate systems, effect of substrate concentration, temperature and pH.

Fluorescence spectroscopy: Simple theory, excited state properties, florescence quenching, molecular rulers (FRET), single molecule florescence, applications in biological systems.

ORD and CD spectroscopy: Polarization of light and optical rotation, Optical rotatory dispersion and Circular dichroism, Circular dichroism of nucleic acids and proteins.

Books Recommended:

1. Physical Chemistry for life sciences; 2nd edn.; P. W. Atkins and J.D. Paula; Oxford University Press; 2010.
2. Fundamentals of general Biological Chemistry; 4th edn.; John . R. Holum; Wiley; 1990.
3. Principles of biochemistry; 3rd edn.; David. L .Nelson, Michael .M.Cox; Worth Pub.; 2002.
4. Physical Chemistry, Principles and applications in biological systems. 4thedn. Tinoco, Sauer, Wang, Puglisi. Pearson education, 2007.
5. Biophysical Chemistry; 2ndedn.; Alan Cooper; RSC. Publishing; 2011.

Course No: CH17209OE
Title: Chemistry of Bio-molecules (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

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

Oils and Fats: Fatty acids and Triglycerides. Saturated and Unsaturated fatty acids (MUFA and PUFA). Rancidity of Oils & Fats. Absorption of toxic substances by fat.
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.
Minerals: Macro and Micro minerals. Their functions and diseases caused by their deficiencies.

Books Recommended

1. Organic Chemistry; 5th edn;. Vol.2,1.L. Finar (Addison Wesley Longman-2000).
2. Biochemistry, Biotechnology and Clinical Chemistry of Enzymes; Trevor Palmer (EWP). Organic Chemistry by I.L.Finar; Vol. II (ELBS Longamnn).
3. Lehninger's Principles of Bio-chemistry; D.L. Nelson; M.Cox Worth publications; 2000.
4. Introduction to Nucleic Acids and Related Natural Products; Ulbight; Oldborn Press.
5. Chemsitry of Natural Products; S.V. Bhat, B.A. Nagasampagi, M. Siva Kumar. Naroosa Publishing House; New Delhi.

Course No: CH17401CR
Title: Organo-Transition Metal Chemistry (04 Credits)

Max. Marks: *100* | ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Sigma Bonded Organometallic Compounds: (16 Contact hours)

Classification, Stability, Comparison to main Organometallic Compounds, Routes of synthesis, Reactions. Decomposition Pathways: Choice, α and β hydrogen transfer. Intramolecular elimination of alkane, Cyclometallation, Stability from bulky substituents, Agostic alkyls, Umpolung.Metal Hydride Complexes: Synthesis, Characterization and Chemical reactions, Non-classical Hydrides (Kubas complexes).

Unit-II Pi-bonded Organometallic Compounds: (16 Contact hours)

Classification, Structure and bonding in Metal- alkene, alkyne, allyl, 1,3-butadiene and Cyclobutadiene Complexes.

Sandwich Compounds: Characteristics; Classification, Synthesis, Reactions, 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.

Unit-III Catalytic Processes involving Transition Metal Organometallic Compounds: (16 Contact hours)

Mechanistic aspects: Oxidative addition, Insertion reactions Reductive elimination and water gas shift reaction (WGSR).

Catalytic mechanism of Hydrogenation, Hydroformylation, Oxidation and Isomerization of alkenes; Olefin metathesis.

Fischer-Tropsch Synthesis and Ziegler Natta polymerization of alkenes.

Asymmeteric and supported Organometallic Catalysis (brief idea)

Unit-IV Fluxional Organometallic Compounds and Synthetic Reactions involving Organo- metallics (16 Contact hours)

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 η^1 Cyclopentadienyls and η^3–allyls.

Stereochemical non rigidity in case of coordination numbers- 4 & 5 (cis-trans, atomic inversion, Berry Pseudorotation).

Synthetic Reactions involving Organo- metallics:

Reactions of coordinated ligands, carbon monoxide, alkyls, alkenes (Green, Mingo's rules). Activation of small molecules: Carbon monoxide, Carbon dioxide and Alkanes.

Role of organo-iron as synthons, Carbon-Carbon coupling and its reactions (Suzuki and Heck).

Books Recommended:

1. The Organometallic Chemistry of Transition Metals; 2nd edn; Robert. H . Crabtree; Wiley; 1994.
2. Fundamental Transition Metal Organometallic Chemistry; Luke hart; Brooks / Cole; 1985.
3. Organometallic Chemistry; 2nd edn ; Mehrotra & Singh ; New age international 2000
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 press 1983.
9. Reaction Mechanism of Inorganic and Organometallic systems; 2nd edn.; Robert .b. Jordan 1998.
10. Inorganic Chemistry ; 4th edn.; Huheey ; E. Keiter & R. Keiter; Addison-Wesley ;1983
11. Modern Inorganic Chemistry; William. A. Jolly; McGraw Hill; 1985.

Course No: CH17402CR
Title: Photo-Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Basics of Photo-Chemistry (16 Contact hours)

Absorption; mechanism of absorption of light

Transition moment integral, Einstein's treatment, molar integrated absorption intensity, natural radiative lifetime & the calculation of life times.

Excitation; d-d transition, charge transfer & intraligand 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 diagramsdepicting excited states.

Frank Condon principle, shapes of absorption & emission bands.

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

Tools and Technique: Light source, measurement of light intensity, chemical actinometry. Flash photolysis.

Unit-II The Chemistry of Excited State Molecules (16 Contact hours)

Photochemical laws & quantum yield. Kinetics & quantum yield of photo-physical (radiative) and photo-chemical processes. Photochemical processes: primary, secondary, adiabatic & non- adiabatic. Properties of thexi states; Determination of dipole moments & acidity constants of excited state molecules.

Photosubstitution and photo reduction of Co (III) complexes.Photosubstitution reaction of Cr (III) and Rh (III) complexes.

Organometallic-Photochemistry: Reactions of metal carbonyls, cleavage of metal-metal bond.

Unit-III Redox Reactions by Excited Metal Complexes (16 Contact hours)

Energy transfer under conditions of weak and strong interaction. Excited state electron transfer. Marcus-Hush model.Conditions of the excited states to be useful as redox reactants. Photochemical electron transfer, [Ru (bipy)3]2+ and [Os (bipy)3]2+.

Photochemical supramolecular devices: devices for photo-induced energy or electron transfer, Devices for information processing, photo-chemically driven molecular machines.

Unit-IV Solar Energy-Prospects and Challenges (16 Contact hours)

Solar energy storage, solar energy conversion, Metal complex sensitizers and electron relays in photochemical splitting of water, Nitrogen fixation and CO_2 reduction. Inorganic photolithography.

Supramolecular photochemistry in natural systems: photosynthesis, bacterial photosynthesis and artificial photosynthesis.

Books Recommended:

1. Reaction Mechanisms of Inorganic and Organometallic Systems; 2nd edn.; Jordon; Oxford; 1998.
2. Mechanism of Inorganic Reactions; Katakis, Gordon; Wiley; 1987.
3. Inorganic Chemistry; 4* edn; Huheey; Harper & Row; 1990.
4. Mechanism of Inorganic Reactions, 2nd edn, Basalo, Pearson; Wiley Eastern, 1997.
5. Chemistry of Light; Suppan, Royal Society; 1994.
6. Photochemistry, Carol J. Wayne and Richard P. Wayne; Oxford University Press; 1996.
7. Fundamentals of Photochemistry; C Rohatgi, Mukhergi; Wiley Eastern.; 1992
8. Inorganic Photochemistry; J.Chem Edu.;Vol .60, No.10,1983.
9. Applications of Inorganic Photochemistry; J. Chem. Edu.; Vol.74, No 69. 1997.

Course No: CH17403CR
Title: Bio-Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Iron Storage, Transport and Oxygen carriers: (16 Contact hours)

Structure and Coordinating sites in biologically important ligands: Proteins, Nucleotides and Lipids.

The transport mechanism: uniport, symport and antiport.

Ferritin and Transferrin: Structure, Metal binding sites; incorporation and release of iron.

Porphyrins: Introduction, characteristic absorption spectrum and salient characteristics.

Haemoglobin and Myoglobin: Structure, oxygen saturation curves; Mechanism of oxygen transport and storage.Bohr effect and cooperativity in haemoglobin.

Hemerythrin and Hemocyanin: Structure, Metal binding groups and Dioxygen binding. Synthetic oxygen carrier model compounds: Vaska's iridium complex: Cobalt complexes with micro and macrocyclic ligands and Schiff base ligands.

Unit-II Metallo-enzymes and Electron Carriers (16 Contact hours)

Enzyme, Apoenzyme, Coenzyme, Prosthetic group and Metalloenzymes, Mechanism of enzyme action.

Zinc enzymes:- Carboxypeptadiase and Carbonic Anhydrase : Introduction, Structure, Mechanism of action and their model compounds.

Biological chemistry of Molybednum: uptake of Molybednum; oxidation states and redox potentials in enzymes and oxygen atom transfer reactions.

Xanthine oxidase and Aldehyde oxidase: Structure and biological role.

Cobalt in Vitamin B_{12}: Introduction, Structure and Derivatives of B_{12} and mechanism of alkylation reaction. Role of vitamin B_{12}.

Electron Carriers: Rubredoxin & Ferridoxin (Structure and biological role).

Blue Copper proteins: Oxidases and Plastocyanin (Structure and biological role).

Unit-III Metal-ion Induced Toxicity and Chelation Therapy (16 Contact hours)

Toxic levels of different metals. Sources of metal ion poisoning (external sources and internal disorders).

Mechanism of metal ion induced toxicity:- Toxicity of Pb, Cd, Hg, As, and CN- Metal ion promoted Carcinogenesis and probable mechanism of action.

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 Metal Salts and Metal Complexes in Therapeutics (16 Contact hours)

Treatment of essential metal deficiencies: Iron, Copper and Cobalt.Metal salts as anti-acids, antiseptic and diuretics.

Gold compounds and Rhematoid arthiritis.

Anti-Cancer Drugs: cis-Platin and its derivatives. Structure-function relationship.

Complexes of Rhodium, Gold and Cobalt.

Anti-bacterial, Anti-viral and Anti-fungal activities of Metal Complexes: Labile and Robust metal complexes; Probable mechanism of action.

Books Recommended:

1. As listed for Course No. CHM—101 (Inorganic chemistry-M.Sc. 1st Semester! From serial No. 1 to 5.
2. Bio inorganic Chemistry -An introduction; Ochai, Allyn and Bacon; 1977.
3. Inorganic Bio-chemistry—Vol. 1&2; Eichhorn; Elsevier, 1973.
4. Inorganic Aspects of Biological and Organic Chemistry; Hanzilik; Academic; 1976.
5. The Inorganic Chemistry of Biological processes; 2nd edn.; Hughes ; Wiley; 1973.
6. A Text book of Medicinal aspects of Bio inorganic Chemistry; Das; CBS; 1990.
7. The Biological Chemistry of Elements; Frausto de Silva; Williams; Clarenden; 1991.
8. Principles of Bio inorganic Chemistry; Lippard, Berg; Univ. Science Books; 1994.
9. Inorganic Chemistry in Biology; Wilkins C & Wilkins G; Oxford; 1997.
10. Bio inorganic Chemistry ; K. Hussain Reddy; New Age International (P) Ltd; 2005.
11. Metal -Ions in Biochemistry; P. K. Bhattacharya; Narosa Publishing House; 2005.

Course No: CH17404CR
Title: Heterocyclic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Structure and Nomenclature of Heterocyclic compounds (16 Contact hours)

Introduction and significance of heterocycles in day to day life.

Nomenclature of Heterocycles: Monocyclic, bicyclic and polycyclic heterocycles, Hantzsch-Widman and replacement methods of nomenclature.

Structural features: Non-aromatic, aromatic and heteroaeromatic heterocycles.

Tautomerism in heterocycles, Meso-ionic systems.

Spectroscopic properties of heterocycles (UV,Visible and ^{1}HNMR).

Unit-II General Approach to Synthesis of Heterocyclic compounds (16 Contact hours)

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 quinoline, Bischler-Napieralki Isoquinoline,Knorr Pyrrole,Paal-Knorr , Fischer – Indole synthesis.

Unit-III Monocyclic Heterocycles (16 Contact hours)

Structure, Synthesis and Reactions of Oxirane, Thirane, Azetidine, Pyrrole, Furan, Thiophene, Diazenes, Pyrimidines,Pyridine.Chemistry of five membered heterocycles with two heteroatoms like 1,3-Azoles, 1,2- Azoles. Chemistry of Six membered rings like Azines and seven membered heterocycles like Azepine,Oxipene,Thiepins.

Unit-IV Bicyclic Heterocycles (16 Contact hours)

Structure, Synthesis and reactions of Benzo- fused heterocycles like Benzo-pyrrole, Benzo-furan,Benzo-thiophene, Quinoline, Isoquinoline, Chromones, Coumarins, Iso-Coumarins, 2 and 4-benzopyrones, Benzopyryllium salts and purines.

Books Recommended:

1. Heterocyclic Chemistry, 5th Ed. J.A.Joule and K.Mills, (Wiley-2010).
2. Essentials of Organic Chemistry, Paul M Dewick , (Wiley-2006).
3. Heterocyclic Chemistry, J.A. Joule and G.F.Smith , (Chapman and Hall-1996).
4. The Chemistry of Heterocycles Theophil Eicher and Siegfried Hauptmann , (George Thieme Verlag Stutt gart,New York -1995).
5. Heterocyclic Chemistry, Raj K. Bansal, (New Age International Publisher-2006).
6. Heterocyclic Chemistry, R.R.Gupta,M.Kumar,V.Gupta,(Springer-2006).

Course No: CH17405CR
Title: Chemistry of Natural Products (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Terpenoids and Carotenoids (16 Contact hours)

Introduction, classification, general methods of isolation, separation.

Essential oils: Separation using Gas Liquid Chromatography and High Performance Liquid Chromatography. Physical, chemical and spectral methods of structure elucidation.

Structure determination, stereochemistry and synthesis of α-terpineol, abietic acid and β-carotene.

Unit-II Alkaloids (16 Contact hours)

Introduction, classification, nomenclature, qualitative tests, pharmaceutical applications and general methods of isolation. Physical, Chemical & Spectral methods of structure elucidation.

Stereochemistry, synthesis and biosynthesis of Quinine, Morphine and Reserpine.

Unit-III Steroids (16 Contact hours)

Introduction, nomenclature, classification & stereochemistry. Physical, Chemical & Spectral methods of characterization. Qualitative tests.

Cholesterol: Isolation, clinical significance, chemical properties, structure elucidation, total synthesis & relationship with bile acids.

Sex hormones: Introduction, isolation, clinical & commercial significance, color reactions, structure determination and partial synthesis of Oesterone, Androsterone, Testosterone and Progesterone.

Glucocorticoids & Mineral Corticoids: Introduction and partial synthesis of Cortisone, aldosterone and synthesis of cholecalciferol.

Unit-IV Natural Plant Pigments and Porphyrins (16 Contact hours)

Introduction, classification, physical, chemical, degradative and spectral methods of structure determination and biosynthesis (Acetate and Shikimic acid pathway)

Flavonoids: Isolation, separation and quantification. Antioxidant activity of flavonoids. Robinson's synthesis, Baker Venketraman synthesis, Kostanecki synthesis of flavanone and Flavanol.

Isolation, structure determination and synthesis of Cyanidin, Chrysin, Quercitin & Genestein.

Porphyrins: Structure determination and total synthesis of haemoglobin. Structural comparison with chlorophyll.

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. New Trends in Natural Product Chemistry, Atta-ur-Rahman (Harward Academic Press).
4. Chemistry of Natural Products, N.R. Krishnaswamy (University Press-1999).
5. Flavanoids; Oyvind M. Andersen and Kenneth R. Markhan. (Taylor & Francis -2006)

Course No: CH17406CR
Title: Bio-Organic and Medicinal Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

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

Vitamins:_ Source, structure and synthesis of vitamins – Vitamin A, Vitamin B-Complex (Thiamine riboflavin, folic acid); Vitamin B-12 (Structure only) Vitamin C, E, K, H and D.

Prostaglandins : Introduction and nomenclature, approaches to prostaglandin synthesis, cyclo-hexane, precursors-Woodward synthesis of PGF2a. Cyclo-heptane precursors - Corey's synthesis of prostoglandin's E & F.Their relationship with oxygenase I and II.

Nucleic Acids: Structure of nucleotide, nucleosides, RNA and DNA, role of nucleic acids in protein synthesis, genetic code and heredity. DNA finger printing

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

Enzymes : Introduction, nomenclature & classification.. Activation & inhibhion of enzymes. Mechanism of enzyme action- Fischer lock and key, koshlands induced fit hypothesis, displacement reactions & coupling of ATP. Enzyme mechanism of chymotrypsin lysozyme & carboxypeptidase.

Co-Enzymes: Cofactors derived from vitamins, coenzymes, prosthetic groups. Apoenzyme. Structure , biological function and mechanism of reactions catalsed by co-enzymes: coenzyme A, thiamine pyrophosphate. pyridoxal phosphate, NAD+, NADP+, FMN, FAD and Lipoic acid.

Unit-III **(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, carbonylic, thiols sulphides groups and introdction/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. Lipophillic constant, Hamett constant, steric parameters and Hansch analysis.

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

Antibiotics: Classifications-structural and mechanistic, cell wall biosynthesis inhibitors, protein synthesis inhibitors. Pencillins-classification and structures. Synthesis of Pencillins, V, G, chloroamphenicol.and ciprofloxacin. Tetracyclins.

Psychoactive Drugs: Introduction, CNS depressants, CNS stimulants, sedatives and hypnotics, barbutirates. Synthesis of diazepam, phenytoins and glutethisimide.

Anti-neoplastic drug: Introduction; cancer chemotherapy, carcenoolytic antibiotic, plant derived anti-cancer agents (Taxol)role of alkylative agents and antimetabolites in treatment of cancer, mitotic inhibitors (elementary idea).

Cardiovascular Drugs: Introduction, cardiovascular diseases, synthesis of Amylnitrate. sorbitrate, quinidine, verapanil, methyl dopa and atenolol

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, Biotechonolgy and Clinical Chemistry of Enzmyes. Trevor Palmer (EWP)
5. Organic Chemistry by I.L.Finar Vol. II (ELBS Longamnn)
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. Chemsitry of Natural Products. S.V. Bhat, B.A. Nagasampagi, M. Siva Kumar. Naroosa Publishing House, New Delhi.

Course No: CH17407CR
Title: Advanced Quantum Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Electronic Structure Theory, Hartree-Fock Method (16 Contact hours)

Review: Electronic Hamiltonian, antisymmetrized wave function, Slater determinant. Hartree-Fock self-consistent field method. One and two-electron integrals in the light of minimal basis H_2 system.

Hartree-Fock Equation, Fock, Coulomb and exchange operators and integrals, restricted Hartree-Fock formalism, Roothaan equation. The Fock matrix elements, Koopman's theorem, Slater-Condon rules. Matrix form of Roothaan equation, the SCF procedure.

Basis Sets: Slatter-type orbitals, Gaussian basis sets. Model SCF calculations on H_2 /$HeH^{+.}$

Unit-II Configuration Interaction and Semiempirical methods (16 Contact hours)

Configuration Interaction: Electron correlation, configuration state functions, configuration interaction (CI), Brillouin theorem, full and truncated CI theories- CID, CISD, CISDTQ methods; Size consistency problem. Moller-Plesset and Coupled Cluster methods.

Semiempirical methods: The ZDO approximation; the PPP method, brief idea of CNDO, INDO and NDDO methods. The MINDO, MNDO, AM1 and PM3 methods.

Unit-III Density Functional Methods and Molecular Properties (16 Contact hours)

Density Functional Theory:Electron probability density. Hohenberg-Kohn theorems, Kohn-Sham formulation of DFT, n- and v- representabilities, E_x&$E_c$functionals; the local density and local spin density approximations, gradient corrected and hybridfunctionals.

Brief idea of Molecular mechanics methods, force fields.

Molecular Properties*:* Potential energy surfaces; molecular geometry and its optimization, Hessian Matrix and normal modes, vibrational frequencies, thermodynamic properties. Dipole moments, atomic Charges.

Unit-IV Use of Quantum Chemistry Software: Gaussian (16 Contact hours)

A quick tour of GAUSSIAN Interface. Input to Gaussian. Model calculations illustrating various features of the package**..**

1. A single point energy calculation: HCHO /CH3.CHO,HCHOMOs.
2. Geometry Optimization: Input and Output for ethene, fluoroethene, propene conformers
3. Transition state optimization $CH_2O \rightarrow HCOH$
4. NMR properties of ethane, ethene and ethyne.
5. Frequency Calculations: Input, Formaldehyde frequencies, Normal modes, zero point energy, thermodynamic properties, polarizability, hyperpolarazability.
6. Stationary points characterization –C3H5F
7. Model Chemistries: Basis set effect on HF bond length

8. Selecting an appropriate theoretical method:
   a) Electron correlation and post SCF methods, limitations of Hartree-Fock theory: HF bond energy, Optimization of O_3.
   b) Density Functional Theory: CO_2 structure and atomization energy.
   c) Butane / Isobutane isomerization energy, rotational barrier in n-butane.

9. Chemical reactions and reactivity:
   a) Hydration enthalpy of the reaction $H^+ + H_2O \rightarrow H_3O^+$
   b) Potential energy surfaces. Reaction path following (IRC calculation)
   $CH_2O \rightarrow HCOH$
   c) Heat of formation of CO_2 via an isodesmic reaction
10. Solvation models: Formaldehyde Frequencies in Acetonitrile

Books Recommended

1. Quantum Chemistry, Ira. N. Levine, (Prentice Hall, 2009).
2. Quantum Chemistry, 2nd Edn , D. A. McQuarrie, (University Science Books, 2007).
3. Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedmann, (Oxford, 2008).
4. Quantum Chemistry and spectroscopy, Engel & Reid, Pearson (2007)
5. Modern Quantum Chemistry - Introduction to Advanced electronic structure theory - A. Szabo & N. S. Ostlund, (Macmillan, 1982, Dover 1996).
6. Molecular Modeling, Principles and Applications, A. R. Leach, Prentice-Hall, 2001
7. Modern Electronic Structure Theory, D. R. Yarkouy (ed). (World Scientific, 1995)
8. Ab Initio Molecular Orbital Theory, by Hehre, Radom, Schleyer and Pople, (Wiley)
9. Density Functional Theory of Atoms and Molecules, R.G. Parr and W. Yang, Oxford(1989).
10. GAUSSIAN Manual, Gaussian Inc
11. Exploring chemistry with electronic structure methods, Foresman J.B., Frisch A., Gaussian Inc

Course No: CH17408CR
Title: Advanced Electrochemistry and Statistical Mechanics (04 Credits)

Max. Marks: *100* | ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Instrumental Methods in Electrochemistry (16 Contact hours)

Fundamentals: Electrode potential and its measurement, standard and formal electrode potentials, three electrode measurements, uncompensated resistance.

Overview of electrode Processes: Faradaic and Non-Faradaic processes, factors affecting electrode reaction rate. Mass transfer: Convection, migration, diffusion, Fick's 1st and 2^{nd} law of diffusion,

Electrochemical Techniques:

Electrophoresis: Factors affecting ion migration, electro-osmosis, theory and applications of capillary electrophoresis.

Potential Step Methods: Chronoamperometry, Chronocoulometry at macro electrodes; theory and applications. Cottrell equation. Controlled-Potential coulometry, Constant-Current coulometric titrations.

Potential Sweep Methods: Linear sweep Voltammetry and Cyclic Voltammetry at macro electrodes theory and applications, Diagnostic criteria of Cyclic Voltammetry.

Unit-II Applied Electrochemistry (16Contacthours)

Electrochemistry of redox enzymes: Direct and mediated electron transfer, Enzyme modified electrodes-challenges and applications. Mechanism and approach to bioelectrosynthesis, examples of bioelectro synthesis-oxidation of alcohols, synthesis of dihydroxy acetone phosphate, site specific oxidation of sugars, reduction of carbonyl compounds, hydrogenation.

Energy storage devices: Desirable characteristics of energy storage devices, Discharge plot, Ragone plot. Batteries: Measures of battery performance. Classical batteries (Lead Acid, Nickel-Cadmium, Zinc-Mangenese dioxide). Modern batteries (Zinc-Air, Nickel-Metal Hydride, Lithium Ion Batteries), Supercapacitors.

Fuel cells, types of fuel Cells, basic fuel cell operation, kinetics of fuel cell reactions. Alkaline, Phosphoric acid, Polymer Electrolyte membrane and direct MeOH fuel cell, biofuel cells.

Unit-III Classical Statistical Mechanics and Ensemble concept (16 Contact hours)

Equations of Motion; Newton, Lagrange and Hamiltonian. Classical partition function, phase space and the Liouville equation, Kinetic theory of gases, equi-partition of energy, Maxwell's velocity distribution.

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. Statistical Mechanical treatment of imperfect gases. Virial equation of state from grand

partition function, virial coefficients in the classical limit, second and third virial coefficients.

Unit-IV Applied Statistical Mechanics (16 Contact hours)

Quantum Statistics: Fermi-Dirac and Boson-Einstein statistics, Nuclear spin statistics, symmetry and nuclear spin, Ortho and Para nuclear spin states, Ortho and Para Hydrogen and Deuterium, CO.

Application of grand partition function to Boson-Einstein and Fermi-Dirac statistics. Ideal Fermi-Dirac gas: Electrons in metals, Ideal Photon gas: Black body radiation, influence of wavelength for the Planck distribution, Bose-Einstein condensation.

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. Electrochemical Methods Fundamentals and Applications, 2ndEdition, Allen J.Bard, Larry R. Faulkner, John Wiley and Sons, INC.
2. Physical Electrochemistry-Principles, Methods and Applications, Israel Rubinstein (Ed.) Marcel Dekker, Inc. New York.
3. Understanding Voltammetry, 2nd Edition, Imperial College Press.
4. Elements of Molecular and Biomolecular Electrochemistry, Jean-Michel Saveant, Wiley-Interscience.
5. Electrochemistry, 2nd Edition, Carl H. Hamann, Andrew Hammett, Wolf Vielstich,Wiley-VCH.
6. Modern Electrochemistry 2B, 2nd Edition, J. O`M. Bockris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.
7. Statistical Thermodynamics, M. C.Gupta ,(NewAgeInternational,1993).
8. Statistical Thermodynamics-Fundamentals and Applications, N.M. Laurendeau, Cambridge University Press, 2005.
9. Statistical Mechanics, D.A. McQuarrie, (Viva,2003).
10. Introduction to Statistical Thermodynamics, Chandler, (OUP, 1987).
11. Statistical Thermodynamics and Kinetic Theory, C. E. Hecht, (Dover,1990).
12. Statistical Mechanics –Principles and Applications, Hill, Dover, 1987.
13. Statistical Thermodynamics for Chemists, A. Ben-Naim, (Plenum, 1992).
14. An introduction to Statistical Thermodynamics, Hill, (Addison-wesley,1987).

Course No: CH17409CR
Title: Chemistry of Materials (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Surfactant mixtures, Stimuli responsive surfactants and block copolymers (16 Contact hours)

Surfactant-Surfactant Interactions: Mixed micelle formation, mixed monolayer formation, synergism, Clint and Rubingh's models of mixed micelle formation**.** Importance and practical applications of mixed surfactant systems.

Stimuli-Responsive Surfactants: Introduction and applications: Biosurfactants, redox, photochromic, thermoreversible, pH-sensitive, cleavable and magnetic surfactants.

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

Unit-II Hydrogels and microemulsions (16 Contact hours)

Hydrogels: Introduction, Types of Hydrogels, Preparation, Properties and characterization of Hydrogels, Biomedical applications of Hydrogels.

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

Unit-III Langmuir Blodgett Films, Liquid crystals and Fullerenes (16 Contact hours)

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.

Fullerenes: Fullerenes- History, bonding, properties, doped fullerenes, fullerenes as superconductors and fullerene related compounds (carbon nanotubes).

Unit-IV Optical materials and Ionic conductors (16 Contact hours)

Optical materials: Luminesence and phosphors. Lasers – general principle of lasing action, Ruby laser, Neodymium-YAG lasers, semiconducing lasers and quantum dot lasers. Nonlinear optical effects, second and third order harmonic generation, nonlinear optical materials.

Ionic Conductors: Introduction to ionic conduction and mechanism. Types of ionic conductors, mechanism of ionic conduction, interstitial jumps (Frenkel); vacancy

mechanism. Super-ionic conductors: Diffusion and transition superionic conductors and mechanism of conduction in superionic conductors; examples and applications of ionic conductors.

Books Recommended:

1. M. J. Rosen, J. T. Kunjappu, “Surfactants and Interfacial Phenomena”, John Wiley & Sons, New York, 4th Edition, 2012.
2. R. D. Vold and M. J. Vold, “Colloid and Interface Chemistry”, Addison-wesley, 1982.
3. .D. Y. Meyer, “Surfaces, Interfaces and Colloid”, VCH Publishers, Inc. 1991.
4. Jonsson, Lindmann, Homberg and Kronberg, “Surfactants and polymers in aqueous solution”, John Wiley and sons, 1998.
5. D. Fennell Evans, H. Wennerstrom, “The Colloidal Domain where physics, chemistry, biology and technology meet” VCH, New York, 1994.
6. Robert J. Hunter, “Foundations of Colloid Science”, Oxford University Press, New York, 2007.
7. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
8. I. W. Hamley, The Physics of Block Copolymers (Oxford University Press, Oxford, 1998.
9. N. Hadijichristidis, S. Pispas and G. A. Floudas Block Copolymers (Wiley, New York, 2003).
10. Introduction to Solids, Azaroff, Tata McGraw,1993.
11. SolidState Chemistry and its Applications, West, Wiley,1989.
12. The Physical Chemistry of Solids, Borg, Biens, Academic press, 1992.
13. Solid State Physics, N. W. Ashcroft and N. D. Mermin, Saunders college, 2001
14. Principles of Solid State, H. V. Keer, Wiley Eastern.
15. The Physics and Chemistry of materials, J.I. Gersten, F.W. Smith, John Wiley and sons, Inc. 2001.
16. Microemulsions: Background, New Concepts, Applications, Perspectives, C. Stubenrauch, Blackwell Publishing Ltd, 2009.
17. M. Sirousazar, M. Foroug, K. Farhad, Y. Shaabani and R. Molaei, Hydrogels: Properties, Preparation, Characterization and Biomedical, Applications in Tissue Engineering, Drug, Delivery and Wound Care, IN Advanced Healthcare Materials, Wiley online Library, 2014.

Course No: CH17410DCE
Title: Advanced Laboratory Course in Inorganic Chemistry (04 Credits)

Max. Marks: *100* — ***Duration:*** *64 Contact hours*
External Exam: *75 Marks.* — ***Internal Assessment****: 25 Marks*

A: - Inorganic Preparations: (5 Experiments)

- Preparation of tetraamminecarbonatocobalt (III) nitrate and its conversion to pentaamminecholorocobalt (III) chloride.
- Preparation of trans dicholoro bis (ethylenediamine) cobalt (III) chloride and its conversion to cis-isomer.
- Preparation of tris (ethylenediamine) nickel (II) chloride dihydrate and its conversion to bis (ethylenediamine) nickel (II) chloride.
- Preparation of bis (acetylacetonato) copper (II) dihydrate.
- Preparation of pentaamminecholorocobalt (III) chloride and study of Linkage isomers by its conversion to pentaamminenitritocobalt (III) chloride and to nitro isomer followed by IR Characterization.

B:- Total analysis of a Coordination compound for determination of various components present.

(1- Experiment)

C: - Separation by Column Chromatography and Estimations: (5 Experiments)

- Separation of Permanganate and Bichromate ions on Alumina column and their Estimation from Beer Law plots.
- Determination of lonisable chloride in a Complex by cation exchange column (separation followed by Mohr's titration of elute for estimation).
- Separation of Cobalt (II) and Nickel (II) on anion exchange column followed by estimation through EDTA titrations.
- Separation of two Cobalt (III) complexes viz $[Co(NH_3)_6]Cl_3$ and $[Co(NH_3)_5Cl]Cl_2$ on Silica column.
- Ion exchange separation of Hydration / ionization isomers of Chromium (III) Chloride ($CrCl_3$).

D: - Potentiometric Titrations: (6 Experiments)

- Standardization of an Iron (ii) solution with a standard dichromate solution over Pt & Calomel assembly.
- Determination of purity of Ce (IV) Sulphate with a standard Iron (II) solution over Pt & Calomel assembly.
- Estimation of Iodide with Standard $AgNO_3$ over Pt & Calomel assembly using I^- \ I2 redox couple.
- Simultaneous determinations of Chloride and Iodide ions with Standard $AgNO_3$ over Ag-Glass electrode assembly.
- Determination of the purity of $[Co(NH_3)_5Cl]Cl_2$ over Ag-Glass electrode assembly.
- Complexometric titration for determination of Ferro cyanide with standard Zinc (ii) solution and inorder to establish the composition of the complex $K_2Zn_3[Fe(CN)_6]_2$

E: - pH-metric Titrations: (2 Experiments)

- Quantitative analysis of Chromate Dichromate mixture by pH Titration.
- Purity of Acetyl Salicylic acid (Asprin) in a commercial tablet by pH Titration.

F: - Conductometric Titrations: (2 Experiments)

- To determine the solubility and solubility product of a sparingly soluble salt ($BaSO_4$) in water.
- To determine the basicity of sodium potassium tartarate by Conductometric method.

G:- Spectrophotometry: (5 Experiments)

- Determination of Iron (II) with 1,10-Phenanthroline.
- Determination of Phosphate by Molybdenum blue method.
- Determination of formula of Iron (III) thiocyanate complex by Job's Continuous variation method.
- Determination of composition of Iron (II)—2,2-bipyridyl complex by Mole ratio method.
- Determination of rate of Aquation of complex $[Co(NH_3)_5Cl]Cl_2$ in acidic medium.

H: - Flame Photometry: (2 Experiments)

- Simultaneous determination of Sodium and Potassium in the given mixture.
- Determination of Cadmium and Magnesium in tap water.

Books Recommended:

- Vogel's quantitative analysis 6 Edn. Mendham, Denny; Pearson Education 2002
- Synthesis and Technique in Inorganic chemistry , G. S.Girlomi; R.J. Angleci 3rd edn.; University Science Books.
- Synthesis and characterization of Inorganic compounds W.AJolly
- Inorganic syntheses Vols II, VI Academic Press.
- Experimental Inorganic / Physical Chemistry ; Mounir A. Malati Horwood/1999.
- Quantitative Chemical Analysis ; 5th edn.; Harris ; Freeman ; 1999.
- Advanced Practical Inorganic Chemistry ; Adams ; Raynor, Wiley ; 1995.
- Advanced Experimental Inorganic Chemistry ; Ayodha Singh ; Campus Books 2002.

Course No: CH17411DCE
Title: Advanced Laboratory Course in Organic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *75 Marks.* ***Internal Assessment****: 25 Marks*

1. **Multistep synthesis of drugs/ organic coinpouiuls involving name reactions**
   (1) Synthesis oflocal 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.
2. **Extraction/Estimation of Organic compounds from Natural sources**
   (1) Isolation of lycopene and β-carotene from tomato and their characterization using *uv*- spectroscopy.
   (2) Isolation of limonene from its natural source and physicochemical analysis.
   (3) Assay of Belladona for Hyoscyamine.
   (4) Assay of lemon from citric acid and vitamin-C
   (5) Isolation of cholesterol from gallstone
   (6) Assay of coke (soft drink)
3. **Column Chromatography**
   Separation of two component solid mixture. Identification of separated components using physical, chemical and spectral techniques.
4. **Spcctrophotomctric estimation** (UV/visible)
   (1) Vitamin-C (Ascorbic acid)
   (2) Caffeine from tea.
   (3) Cholesterol
   (4) Aspirin
5. **Elcctrophoresis/ Paper chromatography**
   Separation and identification of aminoacids by elcctrophoresis / Paper chromatography.
6. **Spcctroscopy**
   Identification of Organic compounds through interpretation of their spectra (UV, IR, PMR, CMR and Mass. Spectra to be provided).

Books Recommended :

1. Comprehensive Practical Organic Chemistry, V.K. Ahluwalia, Renu Aggarwal (Univ. Press India Limited -2000).
2. Vogel's Text Book of Practical Organic Chemistry, B.S.Furniss, A. J. Hannaford (AWL 5^{th} Ed.-1998).
3. Organic Laboratory Techniques , Donald .C. Pavia, Gary . M. Lampman (SCP 3rdEd.-1999)
4. Experiment Organic Chemistry, John.C. Gilbert., Stephen.F.Martin (SCP -1998)
5. Advanced Practical Organic Chemistry Vol. II, Jag Mohan (Himalaya Pub. House First Ed.-1992.

Course No: CH17412DCE
Title: Advanced Laboratory Course in Physical Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *75 Marks.* ***Internal Assessment****: 25 Marks*

A. Tensiometry
1. Investigation of variation of surface tension of n-butanol and sodium chloride solutions with concentration and hence determination of their surface excess concentrations using Gibb's Adsorption Isotherm.
2. Determination of CMC value of a detergent using tensiometry.

B. Cryoscopy
1. Investigation of variation of freezing point depression with concentration & determination of molecular mass.
2. Determination of the degree of dissociation of a salt/weak acid in solution.
3. Determination of activity co-efficient from freezing point measurements.

C. Spectrophotometry
1. To study the complexation reaction between Fe(III) & salicylic acid.
2. Determination of pK value of an indicator.

D. Spectrofluorometry
1. To determine the rate constant for fluorescence quenching of anthracene or perylene by CCl_4 in ethanol.
2. Using pyrene as probe determine the cmc of a surfactant and site of solubilization of pyrene in the micelle through spectrofluorometry.

E. Potentiometry
1. Precipitation titration of KCl, KBr, KI and their mixture with $AgNO_3$
2. Thermodynamics of a chemical reaction by EMF-method.
3. Determination of (a) Standard electrode potential & (b) Activity Coefficient.

F. Conductometry
1. Verification of Debye-Huckel-Onsagar law.
2. Precipitation titration of $BaCl_2$ and K_2SO_4/ $(NH_4)_2SO_4$
3. Estimation of the concentrations of H_2SO_4, CH_3COOH and $CuSO_4$ in a mixture.

G. Dynamic Electrochemistry
1. To estimate the surface area of a working electrode through chronoamperometry and chronocoulometry.
2. Using Cyclic Voltammetry to determine the formal potential and diffusion coefficient of $[Fe(CN)_6]^{3-}$.
3. Use cyclic voltammetry to determine the concentration of acetaminophen in a given sample.

H. Kinetics

1. Kinetic Investigation of BZ-Oscillatory reaction.
2. Kinetic study of enzyme catalyzed reaction (effect of pH and Temperature).

I. Viscometry and densitometery

1. Determination of Mol. Mass of a Polymer (Polyv inyl alcohol) using viscosity method.
2. To explore the nature of chemical bonding (head-head and Head tail linkage of monomers) in polyvinyl alcohol using Viscometry.
3. Determination of partial molar volume of sodium chloride solutions as a function of concentration from density measurements.

Books Recommended

1. Practical Physical Chemistry --- Findley revised by Kitchner.(Longman, 1971)
2. Experimental Physical Chemistry, A. M. Halpern, G. C. McBane, (Freeman, 2006)
3. Experiments in Physical Chemistry, 5th ed. --- Schoemaker et al. (MGH, 2003)
4. Experimental Electrochemistry---R. Holze (Wiley-VCH, 2009).

Course No: CH17413DCE

Title: Supramolecular Chemistry (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*

Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Supramolecular Interactions (08 Contact hours)

Definition and Development of Supramoleclar Chemistry. Nature of Supramolecular Interactions.

Hard Soft Acid Base Concept- Concept, Classification, Symbiosis. Utility in drug design and molecular recognition. Soft Ligands for Soft Metal Ions-Mixed Crown Ethers and Mixed Cryptands.

Unit-II Supramolecular Receptors (08 Contact hours)

Cation Receptors: Supramolecular Cation Coordination Chemistry, EDTA- The Supramolecular Host. Introductory account of Cation Receptors - Podands, Corands, Cryptands, Spherands and Calixarenes.

Anion Receptors: Scope and Challenges, Anion Hydrophobicity-Hofmeister Series, Introductory Account of Anion Receptors - Cyclophanes, Pyrolles, Azacrowns and Metal Based receptors. Hydride Sponge and Anticrowns.

Ion-Pair Receptors: Concept and Significance

Unit-III Crystal engineering and Supramolecular Motiffs (08 Contact hours)

Crystal Engineering: Introduction, Tectons and Synthons. Hydrogen Bond- Introduction, Criteria

Nature and Importance.

Self Assembly: Scope and Objectives. Concepts and Classification. Introductory Account of Coordination Capsules, Catenenes, Rotaxenes and Molecular Knots.

Unit-IV Network Solids and Molecular Devices (08 Contact hours)

Network Solids: Concepts and Classification, Network Topology. Zeolites: Structure, utility and limitations. Metal Organic Frameworks-Introduction and application in catalysis and Gas storage.

Molecular Devices**:** Philosophy of Molecular Devices, Photophysical Fundamentals and Mechanism of Energy and Electron Transfer, Introductory Account of Molecular Wires, Molecular Switches and Molecular Motors.

Books 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, Ist 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. Chemical Reviews. Vol. 115, Issue 15, year **2015**, Pages 6999-8156
8. Introduction: Supramolecular Chemistry. F. Huang and E. V. Anslyn. Chem. Rev. **2015**, 115, 6999−7000.
9. Supramolecular materials. D. B. Amabilino, D. K. Smith and J. W. Steed. Chem. Soc. Rev., **2017**, 46, 2404—2420
10. A Bond by Other Name. G. R. Desiraju. Angew. Chem. Int. Ed. **2011**, 50, 52-59.
11. The Weak Hydrogen Bond: In Structural Chemistry and Biology. G. Desiraju, T. Steiner. **Oxford, IUCr Monograph on Crystallography**.

Course No: CH17414DCE
Title: Designing Organic Synthesis (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I (A) Oxidative and Reductive Processes in Organic Synthesis (8 Contact hours)

***Oxidation*:** Introduction, Aromatisation of cycloalkanes and alkenes using metal catalysts and DDQ. Oxidation of Alcohols using chromic acid, DCC and Swern reagent. Oppenaur oxidation. Oxidation of ketones. Oxidation at activated carbon-hydrogen bond. Oxidation with Selenium dioxide. Prevost hydroxylation and its modification by Woodward.

***Reduction*:** lntroduction. Reduction of Alkenes, Alkynes and Aromatic rings.

Reduction of carbonyl compounds: Clemmensen and Wolf-Kishner reductions. Reductions using $LiAlH_4$ and $NaBH_4$ Bouveault-Blanc reduction. Reduction of Epoxides, Nitro, Nitroso, Azo and Oxime groups. Reductions using Tributyl Tin Hydride.

(B) Protection and Interconversion of Functional Groups (8 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-II 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, α, β-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; Verlage VCH;1986.
3. Principles of Organic Synthesis 2nd edn;. R. O. C. Norman; Chapman and Hall; 1978.
4. Advanced Organic Chemistry Part B, 5th edn.; F. A. Carey and R.J Sundberg ; Springer; 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, 6lh Ed., J. March,; Wiley; 2012.
9. Organic Synthesis- The disconnection Approach; Sturat Warren; Wiley; 2013

Course No: CH17415DCE
Title: Computational Chemistry (02 Credits)

Max. Marks: *50* — ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I

(a) Numerical solution of equations **(8 Contact hours)**

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

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

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

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

(b) Numerical differentiation and integration **(8 Contact hours)**

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

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

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

Unit-II

(a) Interpolation and Curve Fitting **(8 Contact hours)**

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

Lagrange's interpolation method, Newton's divided differences, Cubic spline, piece wise interpolation.

Least squares approximation, linear and quadratic.

(b) Use of Mathematica/Scilab for numerical solution of problems(8 Contact hours)

The mathematica package will be used for the solution of problems covered under the above three units.

Books Recommended

1. Data Reduction & Error Analysis, Bevington& Robinson, (McGraw-Hill, 2003)
2. Computational Chemistry, A. C. Norris, (Wiley.)
3. Computer Software Applications in Chemistry - P. C. Jurs, (John Wiley, 1996.)
4. Numerical Methods for Scientists and Engineers, H. M. Antie, (TMH,).
5. Numerical Recipes in Fortran/C, W.H. Press et al., (CUP,1992)
6. Applied Numerical Analysis, Gerald &Wheatly, (Pearson Education, 2002)
7. Mathematical Methods for Scientists and Engineers, D.A. McQuarie, Viva Books, 1st Ed., 2009.
8. Mathematica Manual.

Course No: CH17416DCE
Title: Seminar (02 Credits)

Presentation by a candidate on any topic chosen in consultation with the teacher incharge.

(25 Marks)

Manuscript (on the topic) submission (25 Marks)

Course No: CH17417GE
Title: Synthetic Polymers and their Applications (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

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

Course No: CH17418GE
Title: Novel Materials (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

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

Block Copolymers: Introduction: classification, micellization of diblock 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, photoconductivity and sensors.

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

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

Luminesence and phosphors. Lasers - general principle of lasing action, Ruby laser, semiconducing 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 Nanofluids 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, Jeremy Ramsden and Ventus Publishing ApS, 2009.

Course No: CH17419OE
Title: Food Chemistry (02 Credits)

Max. Marks: *50* — ***Duration:*** *32 Contact hours*

Ist Unit Exam: *25 marks* — ***IInd Unit (Term end) Exam:*** *25 marks*

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_2, 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; 3rd Ed.; Marcel Dekker, Inc. NY; 2005.
2. Food: The Chemistry of its components; T.P. Coultate; 3rd 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; 2nd ed.; Springer International Edition; 2005.

Course No: CH17301CR
Title: Selected Topics in Inorganic Chemistry (04 Credits)

Max. Marks: *100* | ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit Exam:*** *25 marks*
End Term Exam (Units III & IV): *50 Marks*

Unit-I Metal-ions in Biological Systems: (16 Contact hours)

The role of metal-ions in Metal-Protein systems; in trigger and control mechanisms; in structural context; as Lewis acid and as redox catalysts.
Biodistribution and biochemical role of essential trace and ultra-trace elements:- Fe, Zn, Cu, V, Cr, Mn, Ni, P, F and I. Effects of their deficiencies and treatment.
Antagonism and Synergism among essential trace elements.
Alkali and Alkaline earth metal ions (Na^+, K^+, Ca^{2+} & Mg^{2+}): Biological role; ligands and mechanism of ion transport (Facilitated transport, Carriers, Channeling and active transport of Cations).
Role of Lithium in mental health.
Chlorophyll: Structure and role of magnesium in photosynthesis.
Biological Nitrogen Fixation: Dinitrogen Complexes and their reactivity; Nitrogenase enzyme; Fixation via nitride formation.

Unit-II Bonding in Main Group Compounds (16 Contact hours)

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 Compounds (Borazine), Phosphorous–Nitrogen compounds (Cyclophosphazenes, polyphosphazenes and phosphonitrillic halides), Sulphur-Nitrogen compounds (polythiazyls and Sulphur Nitrides)

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 μ_s and μ_{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.
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.

Unit-IV NQR & Mossbauer Spectroscopy. (16 Contact hours)

Basic principles, Spectral parameters such as isomer shift, quadrupole splitting and magnetic splitting, spectrum display.

Application of the technique to the studies of (i) bonding and structure of Fe^{2+} and Fe^{3+} compounds including those of intermediate spin, (ii) Sn^{2+} and Sn^{4+} compounds— nature of M—L bond, coordination number and structure, (iii) detection of oxidation state and inequivalent MB atoms.

NQR isotopes, Nuclear quadruple moment; Electric field gradient; nuclear quadruple coupling constant; Effect of applied magnetic field, Applications.

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; IInd 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. Infrared and Raman Spectra: Inorganic and Coordination compounds ; K. Nakamoto; Wiley.
11. NMR, NQR and Mossbauer Spectrascopy in Inorganic Chemistry ; R.V.Parish; Ellis Horwood.

Course No: CH17302CR
Title: Organic Chemistry (Spectroscopy & Photochemistry) (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (Units III & IV): *50 Marks*

Unit-I Applications of Spectroscopy: (16 Contact hours)

Recapitulation of UV, IR Spectroscopy, Woodward-Fieser rule Characteristic absorptions of various functional groups. Interpretation of IR Spectra.

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. Mass Analyzer Determination of Molecular Formula, Role of Isotopes, Nitrogen Rule, Metastable Peak. Fragmentation pattern like Stevenson rule , initial ionization event, α-cleavage, inductive cleavage, two bond cleavage, Retro-Diels. Alder cleavage, McLaffertey Rearrangements. Fragmentation pattern of alkanes, alkenes, alcohols, phenols, aldehydes, ketones, Carboxylic acids, Amines, Problems based on Mass Spectroscopy. Some specific examples from natural products like flavanoids terpenes, steroids, alkaloids.

Unit-II Nuclear Magnetic Resonance 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 A_2, AB, AX, AB_2, AX_2, A_2B_2. Proton exchange, deuterium exchange, Peak broadening exchange

C-13 NMR : Carbon 13-chemical shifts , proton coupled and decoupled spectra. Nuclear overhouser, Effect, Off-Resonance De-coupling, A quick dip in to DEPT-45 , DEPT-90, DEPT-135.

Introduction to two-dimensional spectroscopy methods, Cosy techniques, HETCOR technique, OESY, combined structure problems.

Unit-III Photochemistry-I. (16 Contact hours)

Photochemical Reactions

Interaction of electromagnetic radiation with matter. Types of excitations. Singlet and triplet states and their lifetimes. Fate of excited molecule: Physical and chemical processes. Transfer of excitation energy: Sensitization and Quenching. Quantum yield. Types of photochemical reactions.

Photochemistry of alkenes

Geometrical isomerisations, cyclisation and dimerisation reactions. Photochemical reactions of 1,3- butadiene (excluding pericyclic reactions). Rearrangements of 1,4 and 1,5- dienes.

Photochemistry of saturated carbonyl compounds

Intramolecular reactions of saturated acyclic and cyclic carbonyl compounds. (Norrish type-I and Norrish type-II processess). Intermolecular cycloaddition reactions (Paterno- Buchi reaction).

Unit-IV Photochemistry –II. (16 Contact hours)

Photochemistry of unsaturated carbonyl compounds

Photochemical reactions of α, β-unsaturated carbonyl compounds. (H-Abstraction and isomerisation to β, γ-unsaturated carbonyl compounds). Photolysis of cyclic α, β-unsaturated ketones (dimerisation and lumiketone rearrangement) and cyclohexadienones.

Photochemistry of Aromatic compounds

Photoinduced isomerisations of benzene and its alkyl derivatives. 1,2 ; 1,3 and 1,4 photoaddition reactions of benzene. Nueleophilic photosubstitution reactions in aromatic compounds. Photo Fries-rearrangement of aryl esters and anilides.

Miscellaneous Photochemical reaction

Photolysis of organic nitrites and their synthetic utility (Barton reaction).

Photochemistry of vision.

Books recommened:

1. Spectrometric identification of Organic Compounds. 5^{th} Ed., R.M.Silverstein, G.C.Bassler and T.C.Morill. (Jhon 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. Intoductory Photochemistry, A.Cox and T.Kemp (McGraw Hall-1971).
6. Organic Photochemistry, 2^{nd} Ed., J.Coxon, and B.Halton (2^{nd} Ed. Cambridge University press-1987).
7. Fundamentals of photochemistry, Rohtagi & Mukherjee (Wiley Eastern-1992).

Course No: CH17303CR
Title: Physical Chemistry (04 Credits)

Max. Marks: *100* — ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit Exam:*** *25 marks*
End Term Exam (Units III & IV): *50 Marks*

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 pi-bond-order. Alternant hydrocarbons, Naphthalene. 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-Fockself consistent field method. One and two-electron integrals in the light of minimal basis H_2 system

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 Electrochemistry-I (16 Contact hours)

Conductance of electrolyte solutions: Mobility of ions, mobility and conductivity, Einstein relations, dependence of molar conductance on concentration, estimation of K and Λ^0 for weak electrolytes, Theories of Conductance: Debye-Huckel-Onsager conductance equation and brief idea of its extension.

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, recent advances.

Semiconductor electrodes: Structure of seminconductor/electrolyte interface.

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

Theories of Heterogeneous Electron Transfer: Electron transfer at electrified interface at and away from equilibrium. Butller-Volmer equation, low and high field approximations, significance of transfer coefficient.

Electrochemistry in Materials Science: Corrosion, types and mechanism of corrosion, corrosion current, corrosion potential, Electrodics of corrosion in absence of Oxide films; Monitoring and inhibition of corrosion; cathodic and anodic protection, passivation.

Photoelectrochemistry: Band bending across Semiconductor/electrolyte solution interface, photoelectrochemistry across semiconductor/electrolyte interfaces, p-type photocathode, n-type-photoanode, surface effects in photoelectrochemitry, photoelectrochemical splitting of water, photoelectrochemical reduction of CO_2.

Books Recommended:

1. Physical Chemistry –P. W. Atkins, 9th Edition, 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, Tata McGraw 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. M. J. Rosen, J. T. Kunjappu, "Surfactants and Interfacial Phenomena", John Wiley & Sons, New York, 4th Edition, 2012.
7. D. Y. Meyer, "Surfaces, Interfaces and Colloid", VCH Publishers, Inc. 1991.
8. Jonsson, Lindmann, Homberg and Kronberg, "Surfactants and polymers in aqueous solution", John Wiley and sons, 1998.
9. Molecular Thermodynamics of Electrolyte Solutions, Lioyd L Lee, World Scientific, 2008.
10. An Introduction to Aqueous Electrolyte Solutions, Margaret Robson Wright, Wiley, 2007.
11. Modern Electrochemistry 1, 2A,2B 2nd Edition, J. O`M. Bokris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.
12. Electrochemical methods, Fundamentals and Methods, A.J. Bard, L.R. Faulkner, Wiley, 1980.
13. Physical Electrochemistry- Fundamentals, Techniques and Applications, Eliezer Gileadi, Wiley-VCH 2011.
14. Electrochemistry, 2nd Edition, Carl H. Hamann, Andrew Hammett, Wolf Vielstich, Wiley-VCH.

Course No: CH17304DCE
Title: Laboratory Course in Physical Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *80 Marks.* ***Internal Assessment****: 20 Marks*

A. Conductometry
1. Determination of the composition of a mixture of HCl and CH_3COOH by titration with standard NaOH.
2. Determination of degree of dissociation of a weak acid.

B. Potentiometry
1. Determination of strength and pKa value of weak acid by titration with an alkali using quinhydrone electrode.
2. Titration of Fe (II) vs. $K_2Cr_2O_7$ and determination of standard redox potential of Fe^{2+}/Fe^{3+}.

C. pH-metry
1. Determination of pKa values of a tribasic acid by titration with an alkali.
2. Determination of degree of hydrolysis of aniline hydrochloride.

D. 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.

E. Spectrophotometry
1. Determination of composition of a binary mixture of $K_2Cr_2O_7$ and $KMnO_4$ or Cobalt (II) and Nickel (II) ions.
2. Spectrophotometric titration of Fe(II) vs. $KMNO_4$.

F. 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.

G. Viscometry
1. Investigation of variation of viscosity with conc. and determination of unknown concentration.
2. Determination of the radius of a molecule by viscosity measurement.

Books Recommended:

1. Practical Physical Chemistry, Findley, Kitchener, Longman, 1977.
2. Advanced Practical Physical Chemistry, Yadav , Goel Pub, 1994.
3. Experiments in Physical Chemistry, 5th ed., Schoemaker et al. , MGH, 1989.

Course No: CH17305DCE
Title: Chromatographic Techniques (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

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; 5th Edition; F. W. Fifield, D. Kealey; Blackwell Sciences Ltd.; 2000.
2. Modern Analytical Chemistry; David Harvey; McGraw-Hill; 2000.
3. Chromatographic Methods; 5th edn. ; A. Braithwaite and F. J. Smith; Kluwer Academic Publishers.
4. Fundamentals of Analytical Chemistry; 6th 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: CH17306DCE
Title: Non-Equilibrium Thermodynamics (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

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 stationery 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 IrreversibleProcesses;DeGroot,Mazur;Dover;1986.
2. Introduction to Thermodynamics of Irreversible Processes; I.Prigogine; Wiley Interscience; 1967.
3. Thermodynamics for students of Chemsitry, Kuriacose, Rajaram, (S. ChandandCo., 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-equlibrium thermodynamics, 2nd ed. Yasar Demirel. Elsevier, 2007.

Course No: CH17307GE
Title: Industrial Pollution and Green Chemistry (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Industrial Pollution and Environmental Toxicology (16 Contact hours)

Industrial Pollution: Cement, Sugar, Drug, Paper and pulp. Thermal power plants, Nuclear power plants and Polymers.

Radio nuclide analysis: Disposal of wastes and their management.

Principles of Toxicology, Dose Response Relationship, risk assessment and management.

Organochlorine Compounds: Accumulation and fate in biological systems. Toxicology of PCBs. Dioxins and Furans, Health effects in humans.

Environmental Estrogens.

Unit-II Green Chemistry (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 and Sonication.

Green Solvents and Reaction conditions: Supracritical fluids, aqueous reaction conditions, immobilized Solvents and irradiative reaction conditions.

Examples of Green materials, reagents and some specific reactions.

Books Recommended

1. Environmental Chemistry; 8th edn.; S. E. Manahan; CRC Press; 2005.
2. Chemistry of the Environment; IInd edn.; T. G. Spiro and W. M. Stigliani; Prentice Hall; 2002.
3. Environmental Chemistry; IInd edn.; Colin Baird; Freeman & Co.; 1991.
4. Chemistry of the Environment; IInd Edn. R. A. Bailey; H. M. Clark; J. P. Ferris; S. Krause & R. L. Strong; Elsevier; 2005.
5. Environmental Chemistry; IInd edn.; Samir K. Banergi; Prentice- Hall; 2001.
6. Green Chemistry- Environment Friendly Alternatives; Rashmi Sangh & M. M Srivastava; Narosa; 2007.
7. Green Chemistry- An Introductory Text; IInd Edn.; Mike Lancaster; RSC; 2010.
8. Green Chemistry- Theory and Practice; P. T. Anastas and J. C. Warner; oxford; 2000.
9. Green Chemistry; Ist Edn.; Samuel Delvin; IVY Publishing House; 2008.
10. Green Chemistry- Environmentally Benign Reactions; V. K. Ahluwalia; Ane Books; 2006.

Course No: CH17308GE
Title: Bio-Organic Chemistry (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I (16 Contact hours)

(a) Chemical Origins of Biology

Bio organic chemistry: Introduction ,Basic consideration , Proximity effects in Organic Chemistry , Molecular rearrangments.

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 Nomeclature 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+ and NADP+), Flavin Nucleotides (FMN and FAD), Adenosine phosphate (ATP, ADP, AMP) .

Coenzyme A (CoA -SH) ,Thiamine Phosphate, Biotin, Tetrahydrofolate, Coenzyme B_{12} .

(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 Gregary Weiss; Taylor and francis. 2013.
2. Bio-organicchemistry : Harman Dugas 3rd ed.Springer (2010) .
3. Bio-organic chemistry J.Rohr ,Springer (2000).
4. Enzymes 2nd ed. T. Palmer and P. Bonner (2008).
5. Biochemistry :Donald Voet, Judith.G. Voet 2nd ed.Willey (1995)

Course No: CH17309OE
Title: Philosophy of Science (02 Credits)

Max. Marks: *50* — ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Representation (08 contact hours)

Laws of nature**:** Knowledge**, S**ources of knowledge, The rationalists, The empiricists, The Mathematical knowledge, Synthetic Knowledge, Science as knowledge source, Religion and science The Method of science, Induction versus deduction, Representation and reason, Probabilistic laws, Basic and derived laws,

Realism: Realism and its critics, Instrumentalism, Constructive empiricism, Laws and antirealism, Anti-realism and structure of science.

Unit-II Reason (08 contact hours)

Inductive Scepticism: Theory and observation, Dissolving the problem of Induction, Probability
and scientific inference, Kinds of Probability,

Inductive Knowledge: Reliabilist epistemology, reasoning with induction, Innate epistemic capacities and reasoning about induction, Internalism and justification.

Method and Progress: Methodology of scientific research programmes, Clinical trials and the scientific method, The content of discovery and the context of justification, Science without the scientific method, Method and the development of sciences, Paradigms and Progress.

Unit-III Classical Determinism and Probabilistic world (08 contact hours)

The Classical Mechanics: Mechanistic determinism, General principles; Action at a distance, Electric and magnetic forces, Failures of the classical mechanics;
Atomic structure, problem of radiation.

The birth of modern science**:** The photo-electric effect**,** The atomicity of radiation, Particle wave duality, waves of probability, Uncertainty principle, subject versus object, the fundamental laws of radioactivity, The new Quantum theory, wave mechanics, Diracs Quantum mechanics, The new philosophical principles, the probabilistic reasoning.

Unit-IV The Dawn of Modern Thinking (08 contact hours)

The arrow of Time: From Descarts to quantum theory, the relation of quantum theory to other natural sciences. Language and reality in modern science. The role of modern science in the present development of human thinking.

Books Recommended:

1. Philosophy of science; Alexander Bird; McGill-Queen's University Press.
2. Physics and Philosophy; W. Heisenberg; Harper Perennial Modern Classics.
3. Physics and Philosophy; Sir James Jeans; Cambridge University Press.
4. Reconstruction of religious thought in Islam; Muhammad Iqbal; Adam Publishers & Dodo Press.
5. Philosophy of natural science; Carl G. Hempel**;** Pearson.
6. The philosophy of science; David Papineaus; Oxford University Press.
7. Reality and Representation; David Papineaus; Blackwell Publication.
8. Belief, truth and knowledge; D.M. Armstrong; Cambridge University Press.
9. Modern epistemology; Nicholas Everitt and Alec Fisher; McGraw-Hill Higher Education.
10. The structure of scientific revolution; Thomas S. Kuhn; The University of Chicago Press

Course No: CH17302CR

Title: Organic Chemistry (Spectroscopy & Photochemistry) (04 Credits)

Max. Marks: *100* — ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit Exam:*** *25 marks*
End Term Exam (Units III & IV): *50 Marks*

Unit-I Applications of Spectroscopy: (16 Contact hours)

Recapitulation of UV, IR Spectroscopy, Woodward-Fieser rule Characteristic absorptions of various functional groups. Interpretation of IR Spectra.

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. Mass Analyzer Determination of Molecular Formula, Role of Isotopes, Nitrogen Rule, Metastable Peak. Fragmentation pattern like Stevenson rule , initial ionization event, α-cleavage, inductive cleavage, two bond cleavage, Retro-Diels. Alder cleavage, McLaffertey Rearrangements. Fragmentation pattern of alkanes, alkenes, alcohols, phenols, aldehydes, ketones, Carboxylic acids, Amines, Problems based on Mass Spectroscopy. Some specific examples from natural products like flavanoids terpenes, steroids, alkaloids.

Unit-II Nuclear Magnetic Resonance 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 A_2, AB, AX, AB_2, AX_2, A_2B_2. Proton exchange, deuterium exchange, Peak broadening exchange

C-13 NMR : Carbon 13-chemical shifts , proton coupled and decoupled spectra. Nuclear overhouser, Effect, Off-Resonance De-coupling, A quick dip in to DEPT-45 , DEPT-90, DEPT-135.

Introduction to two-dimensional spectroscopy methods, Cosy techniques, HETCOR technique, OESY, combined structure problems.

Unit-III Photochemistry-I. (16 Contact hours)

Photochemical Reactions

Interaction of electromagnetic radiation with matter. Types of excitations. Singlet and triplet states and their lifetimes. Fate of excited molecule: Physical and chemical processes. Transfer of excitation energy: Sensitization and Quenching. Quantum yield. Types of photochemical reactions.

Photochemistry of alkenes

Geometrical isomerisations, cyclisation and dimerisation reactions. Photochemical reactions of 1,3- butadiene (excluding pericyclic reactions). Rearrangements of 1,4 and 1,5- dienes.

Photochemistry of saturated carbonyl compounds

Intramolecular reactions of saturated acyclic and cyclic carbonyl compounds. (Norrish type-I and Norrish type-II processess). Intermolecular cycloaddition reactions (Paterno- Buchi reaction).

Unit-IV Photochemistry –II. (16 Contact hours)

Photochemistry of unsaturated carbonyl compounds

Photochemical reactions of α, β-unsaturated carbonyl compounds. (H-Abstraction and isomerisation to β, γ-unsaturated carbonyl compounds). Photolysis of cyclic α, β-unsaturated ketones (dimerisation and lumiketone rearrangement) and cyclohexadienones.

Photochemistry of Aromatic compounds

Photoinduced isomerisations of benzene and its alkyl derivatives. 1,2 ; 1,3 and 1,4 photoaddition reactions of benzene. Nueleophilic photosubstitution reactions in aromatic compounds. Photo Fries-rearrangement of aryl esters and anilides.

Miscellaneous Photochemical reaction

Photolysis of organic nitrites and their synthetic utility (Barton reaction).
Photochemistry of vision.

Books recommened:

1. Spectrometric identification of Organic Compounds. 5th Ed., R.M.Silverstein, G.C.Bassler and T.C.Morill. (Jhon 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. Intoductory Photochemistry, A.Cox and T.Kemp (McGraw Hall-1971).
6. Organic Photochemistry, 2nd Ed., J.Coxon, and B.Halton (2nd Ed. Cambridge University press-1987).
7. Fundamentals of photochemistry, Rohtagi & Mukherjee (Wiley Eastern-1992).

Course No: CH17405CR
Title: Chemistry of Natural Products (04 Credits)

Max. Marks: *100* | ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Terpenoids and Carotenoids (16 Contact hours)

Introduction, classification, general methods of isolation, separation.

Essential oils: Separation using Gas Liquid Chromatography and High Performance Liquid Chromatography. Physical, chemical and spectral methods of structure elucidation.

Structure determination, stereochemistry and synthesis of α-terpineol, abietic acid and β-carotene.

Unit-II Alkaloids (16 Contact hours)

Introduction, classification, nomenclature, qualitative tests, pharmaceutical applications and general methods of isolation. Physical, Chemical & Spectral methods of structure elucidation.

Stereochemistry, synthesis and biosynthesis of Quinine, Morphine and Reserpine.

Unit-III Steroids (16 Contact hours)

Introduction, nomenclature, classification & stereochemistry. Physical, Chemical & Spectral methods of characterization. Qualitative tests.

Cholesterol: Isolation, clinical significance, chemical properties, structure elucidation, total synthesis & relationship with bile acids.

Sex hormones: Introduction, isolation, clinical & commercial significance, color reactions, structure determination and partial synthesis of Oesterone, Androsterone, Testosterone and Progesterone.

Glucocorticoids & Mineral Corticoids: Introduction and partial synthesis of Cortisone, aldosterone and synthesis of cholecalciferol.

Unit-IV Natural Plant Pigments and Porphyrins (16 Contact hours)

Introduction, classification, physical, chemical, degradative and spectral methods of structure determination and biosynthesis (Acetate and Shikimic acid pathway)

Flavonoids: Isolation, separation and quantification. Antioxidant activity of flavonoids. Robinson's synthesis, Baker Venketraman synthesis, Kostanecki synthesis of flavanone and Flavanol.

Isolation, structure determination and synthesis of Cyanidin, Chrysin, Quercitin & Genestein.

Porphyrins: Structure determination and total synthesis of haemoglobin. Structural comparison with chlorophyll.

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. New Trends in Natural Product Chemistry, Atta-ur-Rahman (Harward Academic Press).
4. Chemistry of Natural Products, N.R. Krishnaswamy (University Press-1999).
5. Flavanoids; Oyvind M. Andersen and Kenneth R. Markhan. (Taylor & Francis -2006)

Course No: CH17407CR
Title: Advanced Quantum Chemistry (04 Credits)

Max. Marks: *100* — ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Electronic Structure Theory, Hartree-Fock Method (16 Contact hours)

Review: Electronic Hamiltonian, antisymmetrized wave function, Slater determinant. Hartree-Fock self-consistent field method. One and two-electron integrals in the light of minimal basis H_2 system.

Hartree-Fock Equation, Fock, Coulomb and exchange operators and integrals, restricted Hartree-Fock formalism, Roothaan equation. The Fock matrix elements, Koopman's theorem, Slater-Condon rules. Matrix form of Roothaan equation, the SCF procedure.

Basis Sets: Slatter-type orbitals, Gaussian basis sets. Model SCF calculations on H_2 /HeH^{+}.

Unit-II Configuration Interaction and Semiempirical methods (16 Contact hours)

Configuration Interaction: Electron correlation, configuration state functions, configuration interaction (CI), Brillouin theorem, full and truncated CI theories- CID, CISD, CISDTQ methods; Size consistency problem. Moller-Plesset and Coupled Cluster methods.

Semiempirical methods: The ZDO approximation; the PPP method, brief idea of CNDO, INDO and NDDO methods. The MINDO, MNDO, AM1 and PM3 methods.

Unit-III Density Functional Methods and Molecular Properties (16 Contact hours)

Density Functional Theory:Electron probability density. Hohenberg-Kohn theorems, Kohn-Sham formulation of DFT, n- and v- representabilities, E_x&$E_c$functionals; the local density and local spin density approximations, gradient corrected and hybridfunctionals.
Brief idea of Molecular mechanics methods, force fields.

Molecular Properties*:* Potential energy surfaces; molecular geometry and its optimization, Hessian Matrix and normal modes, vibrational frequencies, thermodynamic properties. Dipole moments, atomic Charges.

Unit-IV Use of Quantum Chemistry Software: Gaussian (16 Contact hours)

A quick tour of GAUSSIAN Interface. Input to Gaussian. Model calculations illustrating various features of the package**..**

1. A single point energy calculation: HCHO /CH3.CHO,HCHOMOs.
2. Geometry Optimization: Input and Output for ethene, fluoroethene, propene conformers
3. Transition state optimization $CH_2O \rightarrow HCOH$
4. NMR properties of ethane, ethene and ethyne.
5. Frequency Calculations: Input, Formaldehyde frequencies, Normal modes, zero point energy, thermodynamic properties, polarizability, hyperpolarazability.
6. Stationary points characterization –C3H5F
7. Model Chemistries: Basis set effect on HF bond length

8. Selecting an appropriate theoretical method:
   a) Electron correlation and post SCF methods, limitations of Hartree-Fock theory: HF bond energy, Optimization of O_3.
   b) Density Functional Theory: CO_2 structure and atomization energy.
   c) Butane / Isobutane isomerization energy, rotational barrier in n-butane.

9. Chemical reactions and reactivity:
   a) Hydration enthalpy of the reaction $H^+ + H_2O \rightarrow H_3O^+$
   b) Potential energy surfaces. Reaction path following (IRC calculation)
   $CH_2O \rightarrow HCOH$
   c) Heat of formation of CO_2 via an isodesmic reaction

10. Solvation models: Formaldehyde Frequencies in Acetonitrile

Books Recommended

1. Quantum Chemistry, Ira. N. Levine, (Prentice Hall, 2009).
2. Quantum Chemistry, 2nd Edn , D. A. McQuarrie, (University Science Books, 2007).
3. Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedmann, (Oxford, 2008).
4. Quantum Chemistry and spectroscopy, Engel & Reid, Pearson (2007)
5. Modern Quantum Chemistry - Introduction to Advanced electronic structure theory - A. Szabo & N. S. Ostlund, (Macmillan, 1982, Dover 1996).
6. Molecular Modeling, Principles and Applications, A. R. Leach, Prentice-Hall, 2001
7. Modern Electronic Structure Theory, D. R. Yarkouy (ed). (World Scientific, 1995)
8. Ab Initio Molecular Orbital Theory, by Hehre, Radom, Schleyer and Pople, (Wiley)
9. Density Functional Theory of Atoms and Molecules, R.G. Parr and W. Yang, Oxford(1989).
10. GAUSSIAN Manual, Gaussian Inc
11. Exploring chemistry with electronic structure methods, Foresman J.B., Frisch A., Gaussian Inc

Course No: CH17401CR
Title: Organo-Transition Metal Chemistry (04 Credits)

Max. Marks: *100* | ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Sigma Bonded Organometallic Compounds: (16 Contact hours)

Classification, Stability, Comparison to main Organometallic Compounds, Routes of synthesis, Reactions. Decomposition Pathways: Choice, α and β hydrogen transfer. Intramolecular elimination of alkane, Cyclometallation, Stability from bulky substituents, Agostic alkyls, Umpolung.Metal Hydride Complexes: Synthesis, Characterization and Chemical reactions, Non-classical Hydrides (Kubas complexes).

Unit-II Pi-bonded Organometallic Compounds: (16 Contact hours)

Classification, Structure and bonding in Metal- alkene, alkyne, allyl, 1,3-butadiene and Cyclobutadiene Complexes.

Sandwich Compounds: Characteristics; Classification, Synthesis, Reactions, 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.

Unit-III Catalytic Processes involving Transition Metal Organometallic Compounds: (16 Contact hours)

Mechanistic aspects: Oxidative addition, Insertion reactions Reductive elimination and water gas shift reaction (WGSR).

Catalytic mechanism of Hydrogenation, Hydroformylation, Oxidation and Isomerization of alkenes; Olefin metathesis.

Fischer-Tropsch Synthesis and Ziegler Natta polymerization of alkenes.

Asymmeteric and supported Organometallic Catalysis (brief idea)

Unit-IV Fluxional Organometallic Compounds and Synthetic Reactions involving Organo- metallics (16 Contact hours)

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 η^1 Cyclopentadienyls and η^3–allyls.

Stereochemical non rigidity in case of coordination numbers- 4 & 5 (cis-trans, atomic inversion, Berry Pseudorotation).

Synthetic Reactions involving Organo- metallics:

Reactions of coordinated ligands, carbon monoxide, alkyls, alkenes (Green, Mingo's rules).

Activation of small molecules: Carbon monoxide, Carbon dioxide and Alkanes.

Role of organo-iron as synthons, Carbon-Carbon coupling and its reactions (Suzuki and Heck).

Books Recommended:

1. The Organometallic Chemistry of Transition Metals; 2nd edn; Robert. H . Crabtree; Wiley; 1994.
2. Fundamental Transition Metal Organometallic Chemistry; Luke hart; Brooks / Cole; 1985.
3. Organometallic Chemistry; 2nd edn ; Mehrotra & Singh ; New age international 2000
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 press 1983.
9. Reaction Mechanism of Inorganic and Organometallic systems; 2nd edn.; Robert .b. Jordan 1998.
10. Inorganic Chemistry ; 4th edn.; Huheey ; E. Keiter & R. Keiter; Addison-Wesley ;1983
11. Modern Inorganic Chemistry; William. A. Jolly; McGraw Hill; 1985.

Course No: CH17409CR
Title: Chemistry of Materials (04 Credits)

Max. Marks: *100* | ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Surfactant mixtures, Stimuli responsive surfactants and block copolymers (16 Contact hours)

Surfactant-Surfactant Interactions: Mixed micelle formation, mixed monolayer formation, synergism, Clint and Rubingh's models of mixed micelle formation**.** Importance and practical applications of mixed surfactant systems.

Stimuli-Responsive Surfactants: Introduction and applications: Biosurfactants, redox, photochromic, thermoreversible, pH-sensitive, cleavable and magnetic surfactants.

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

Unit-II Hydrogels and microemulsions (16 Contact hours)

Hydrogels: Introduction, Types of Hydrogels, Preparation, Properties and characterization of Hydrogels, Biomedical applications of Hydrogels.

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

Unit-III Langmuir Blodgett Films, Liquid crystals and Fullerenes (16 Contact hours)

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.

Fullerenes: Fullerenes- History, bonding, properties, doped fullerenes, fullerenes as superconductors and fullerene related compounds (carbon nanotubes).

Unit-IV Optical materials and Ionic conductors (16 Contact hours)

Optical materials: Luminesence and phosphors. Lasers – general principle of lasing action, Ruby laser, Neodymium-YAG lasers, semiconducing lasers and quantum dot lasers. Nonlinear optical effects, second and third order harmonic generation, nonlinear optical materials.

Ionic Conductors: Introduction to ionic conduction and mechanism. Types of ionic conductors, mechanism of ionic conduction, interstitial jumps (Frenkel); vacancy

mechanism. Super-ionic conductors: Diffusion and transition superionic conductors and mechanism of conduction in superionic conductors; examples and applications of ionic conductors.

Books Recommended:

1. M. J. Rosen, J. T. Kunjappu, "Surfactants and Interfacial Phenomena", John Wiley & Sons, New York, 4th Edition, 2012.
2. R. D. Vold and M. J. Vold, "Colloid and Interface Chemistry", Addison-wesley, 1982.
3. .D. Y. Meyer, "Surfaces, Interfaces and Colloid", VCH Publishers, Inc. 1991.
4. Jonsson, Lindmann, Homberg and Kronberg, "Surfactants and polymers in aqueous solution", John Wiley and sons, 1998.
5. D. Fennell Evans, H. Wennerstrom, "The Colloidal Domain where physics, chemistry, biology and technology meet" VCH, New York, 1994.
6. Robert J. Hunter, "Foundations of Colloid Science", Oxford University Press, New York, 2007.
7. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
8. I. W. Hamley, The Physics of Block Copolymers (Oxford University Press, Oxford, 1998.
9. N. Hadijichristidis, S. Pispas and G. A. Floudas Block Copolymers (Wiley, New York, 2003).
10. Introduction to Solids, Azaroff, Tata McGraw,1993.
11. SolidState Chemistry and its Applications, West, Wiley,1989.
12. The Physical Chemistry of Solids, Borg, Biens, Academic press, 1992.
13. Solid State Physics, N. W. Ashcroft and N. D. Mermin, Saunders college, 2001
14. Principles of Solid State, H. V. Keer, Wiley Eastern.
15. The Physics and Chemistry of materials, J.I. Gersten, F.W. Smith, John Wiley and sons, Inc. 2001.
16. Microemulsions: Background, New Concepts, Applications, Perspectives, C. Stubenrauch, Blackwell Publishing Ltd, 2009.
17. M. Sirousazar, M. Foroug, K. Farhad, Y. Shaabani and R. Molaei, Hydrogels: Properties, Preparation, Characterization and Biomedical, Applications in Tissue Engineering, Drug, Delivery and Wound Care, IN Advanced Healthcare Materials, Wiley online Library, 2014.

Course No: CH17103CR
Title: Physical Chemistry (04 Credits)

Max. Marks: *100* — ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* — ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

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)**

Theories of Chemical Reactions: Activated complex theory of reaction rates, statistical & thermodynamic formulations, comparison with collision theory. Theories of unimolecular reactions (Lindman, Hinshelwood , RRK and RRKM theories), Introduction to potential energy surfaces.

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

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

Unit-IV Chemical kinetics-II **(16 Contact hours)**

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

Reactions in solutions: Diffusion controlled reactions (partial & full microscopic diffusion control), Ionic Reactions; Single & double sphere models of ionic reactions.

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

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

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: CH17204DCE

Title: Laboratory Course in Organic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *80 Marks.* ***Internal Assessment****: 20 Marks*

1. **Qualitative Analyses of Organic Compounds**
   (i) **Physical Properties:** Physical state, colour, odour, solubility behavior 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, Nitrocompounds and Hydrocarbons.
   (iii) **Preparation and recrystallization of the derivatives of above mentioned group of compounds.**
2. **Separation, Purification and identification of Organic compounds from a three component mixture:**
   (a) **Separation based on solubility in water and organic solvents.**
   (b) **Separation based on Chemical properties:** Solubility in Sodium bicarbonate, Sodium Hydroxide and Hydrochloric acid.
   (c) **Identification of individual components using physico-chemical properties**
3. **Detection of functional groups using IR spectroscopy (spectra to be provided)**
4. **Quantitative Estimation of the following compounds**
   (a) Glucose.
   (b) Glycine
   (c) Acetone
   (d) Phenol.
   (e) Ascorbic acid.

5. Organic Preparations

(a) Acetylation of Cholesterol or salicylic acid.

(b) Oxidation of Cyclohexanol by chromic acid to get adipic acid.

(c) Aldol condensation: Dibenzal acetone and benzaldehyde.

(d) Cannizarro's reaction of 4-Chlorobenzaldelyde.

(e) Aromatic electrophillic substitutions in benzene, benzoic acid or aniline.

(f) Beckman rearrangement starting from acetophenone.

(g) Haloform reaction: Preparation of Iodoform.

Books Recommended:

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

Course No: CH17203CR

Title: Physical Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I 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.

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.

Ion solvent Interactions*:* Non structural (Born) treatment and an introduction to structural (Ion-dipole, Ion-quadruple) 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.

Unit-III Biophysical Chemistry (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 (synthesis & hydrolysis), Principles of coupled reactions and their importance for living systems.

Biopolymers: Molecular forces and Chemical bonding in Bio-polymers, hydrophobic interactions, structure of proteins, protein folding and unfolding. Biological membranes, phase transitions in biological membranes. Donan effect and transport across biological membranes.

Binding of Ligands and metal Ions to bio-macromolecules, one binding site per macromolecule, n equivalent binding sites per macromolecule, binding of oxygen to myoglobin and hemoglobin.

Unit-IV Statistical Thermodynamics (16 Contact hours)

Concept of distribution, thermodynamic probability and most probable distribution. Sterling approximation. Method of undetermined multipliers.

Distribution Laws: Derivation of Boltzmann distribution law, Bose-Einstein and Fermi-Dirac laws (without derivation) and their comparison with Boltzmann distribution law.

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

Books Recommended:

1. Physical Chemistry –P. W. Atkins, 9th Edition, 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, Lioyd L Lee, World Scientific, 2008.
7. An Introduction to Aqueous Electrolyte Solutions, Margaret Robson Wright, Wiley, 2007.
8. Modern Electrochemistry 1, 2A, 2nd Edition, J. O`M. Bokris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.
9. Physical Chemistry for the Biosciences, Raymond Chang, University Science Books, 2005.
10. Physical Chemistry for the Life Sciences,2nd Edition, Peter Atkins, Julio de Paula, Oxford University Press2015.
11. Statistical Thermodynamics, M.C.Gupta, New Age International, 1993.
12. Statistical Mechanics, Agarwal, Eisner, Wiley, 1991.

Course No: CH17101CR
Title: Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Stereochemistry and Bonding in the Compounds of Main Group Elements (16 Contact hours)

Valence bond theory: Energy changes taking place during the formation of diatomic molecules; factors affecting the combined wave function. Bent's rule and energetics of hybridization.

Resonance: Conditions, resonance energy and examples of some inorganic molecules/ions.

Odd Electron Bonds: Types, properties and molecular orbital treatment.

VSEPR: Recapitulation of assumptions, shapes of trigonal bypyramidal, octahedral and pentagonal bipyramidal molecules / ions. (PCl_5, VO_3^-, SF_6, $[SiF_6]^{2-}$, $[PbCl_6]^{2-}$ and IF_7).
Limitations of VSEPR theory.

Molecular orbital theory: Salient features, variation of electron density with internuclear distance. Relative order of energy levels and molecular orbital diagrams of some heterodiatomic molecules /ions. Molecular orbital diagram of polyatomic molecules / ions.

Delocalized Molecular Orbitals: Butadiene, cyclopentadiene and benzene.

Detection of Hydrogen Bond: UV-VIS, IR and X-ray. Importance of hydrogen bonding.

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

Stepwise and overall formation constants. Inert & labile complexes. Stability of uncommon oxidation states.

Metal Chelates: Characteristics, Chelate effect and the factors affecting stability of metal chelates.

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-III Bonding 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 ML6; Effect of pi-bonding. Molecular orbital and energy level diagram for bonding in Ferrocene, Square-planar and Tetrahedral complexes.

Unit-IV Pi-acid Metal Complexes (16 Contact hours)

Transition Metal Carbonyls: Carbon monoxide as ligand, synthesis, reactions, structures and bonding of mono- and poly-nuclear carbonyls. Vibrational spectra of metal carbonyls for structural diagnosis.

Prepration, reactions, structure and bonding of transition metal nitrosyls, dinitrogen and dioxygen complexes.

Tertiary phosphine as ligand.

Books Recommended

1. Principles of Inorganic Chemistry; 1^{st} edn.; Brain W. Pfennig; Wiley; 2015.
2. Advanced Inorganic Chemistry; 5^{th}. and 6^{th} edn; F.A. Cotton , G. Wilkinson; Wiley; 1998/1999.
3. Inorganic Chemistry; 4^{th} edn; J. E. Huheey; E. A. Keiter; Harper Collins; 2009.
4. Inorganic Chemistry; G. Wulfsberg; Viva; 2002.
5. Chemistry of the Elements; 2^{nd} edn; N. N. Greenwood, A. Earnshaw; Butterworth; 1997.
6. Inorganic Chemistry; 3^{rd} edn; D. F. Shriver; P. W. Atkins; Oxford; 1999.
7. Inorganic Chemistry; K.F. Purcell, J.C Kotz; Saunders; 1977.
8. Coordination Chemistry; D. Banerjea; Tata McGraw Hill; 1993.

Course No: CH17102CR
Title: Organic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

Unit-I Delocalized Chemical bonding (16 Contact hours)

Overview: Inductive effect. Conjugation, Cross conjugation, Hyperconjugation–Isovalent and sacrificial hyperconjugations, Acids / Bases, Nucleophiles and Electrophiles. Resonance, Rules for writing resonance structures, Steric inhibition of resonance.

Tautomerism: Different types including valence 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.

Unit-II Reactive Intermediates and Determination of Reaction Mechanism (16 Contact hours)

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

Determination of Reaction Mechanism: Reaction Mechanism & Types of reactions. Determining reaction mechanism: Structure of Product, Transition states & Intermediates (Hammond postulate). Catalysis including acid and base catalysis, Specific acid and base catalysis. Fate of individual atoms (Isotope Labeling). Stereochemical course of reaction. Thermodynamic and kinetic evidences. Correlation of structure – reactivity.

Unit-III Stereochemistry: (16 Contact hours)

Chirality: Introduction, Chirality due to chiral centre. Molecules with more than one Chiral centres, Threo and erythro isomers. Convention for of assigning D, L & R, S configurations. Optical activity due to chiral axis, chiral plane and helicity. Chirality involving atoms other than carbon. Chirality in metallic complexes. Enantiotopic and diastereotopic atoms, groups and faces.

Asymmetric Synthesis: Introduction and principle of asymmetric synthesism. Principal categories of asymmetric synthesis. Use of chiral substrates. Diastero-selectivity in Aldol reactions. Sterospecificity and steroselectivity of enzymes.

Confirmations: Origin of conformational energy. Angle and Pitzer strain. Conformational analysis of cycloalkanes, and decalines. Effect of conformation on reactivity in acyclic and cyclic systems. Conformation of sugars & anomeric effect. Conformation of cyclohexene, cyclohexanones and bicycloheptane – a bridged system.

Unit-IV Aliphatic Nucleophilic Substitutions : (16 Contact hours)

Mechanism and stereochemical implications of S_N2, S_N1, S_Ni and Neighbouring Group Participation (by π and σ-bonds) reactions. Comparison of S_N1 and S_N2 reactions. Effect of substrate structure, attacking nucleophile, leaving group and solvent on the rates of S_N1 and S_N2 reactions. Mixed S_N1 and S_N2 reactions. Nucleophilic substitution at allylic, benzylic, aliphatic trigonal and vinylic carbons. Nucleophilic substitution in alcohols, Mitsunobu reactions. Nucleophilic substitutions on other elements. Functional group transformation using S_N2 reactions in organic synthesis. Nucleophilic substitutions in biological systems.

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

Aliphatic Electrophilic Substitutions: General mechanism of S_E1, S_E2 and S_Ei reactions. Mechanisms of reactions involving migration of double bond. Effect of substrate, leaving group and solvent on reactivity. Stork-Enamine reaction.

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 3rd Ed., S.M. Mukherjee and S.P. Singh. (Macmillan-1998).
4. Stereochemistry of Organic Compounds 2nd Ed., D. Nasipuri. (New Age Inter.- 2008)
5. Stereochemistry of Carbon Compounds - E.L.Eliel. (TMH -2007)
6. Stereochemistry of Organic Compounds 7th Ed. - P.S. Kalsi. (New Age Inter.- 2012).
7. Organic Chemistry - 2nd Ed., J. Hornback. (Brooks/Cole- 2006,
8. Organic Chemistry, 5th Ed., John McMurry. (Brooks/Cole-2000).
9. Advanced Organic Chemistry, 5th Ed., F.A Carey & R.J Sundberg (Springer-2007).
10. Organic Chemistry, 2nd Ed., Jonathan Clayden (OUP-2012)
11. Organic Chemistry, 11th Ed., Solomons, T.W.G., (Wiley-2015).

Course No: CH17103CR
Title: Physical Chemistry (04 Credits)

Max. Marks: *100* | ***Duration:*** *64 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit Exam:*** *25 marks*
End Term Exam (units III & IV): *50 Marks*

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)

Theories of Chemical Reactions: Activated complex theory of reaction rates, statistical & thermodynamic formulations, comparison with collision theory. Theories of unimolecular reactions (Lindman, Hinshelwood , RRK and RRKM theories), Introduction to potential energy surfaces.

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

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

Unit-IV Chemical kinetics-II (16 Contact hours)

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

Reactions in solutions: Diffusion controlled reactions (partial & full microscopic diffusion control), Ionic Reactions; Single & double sphere models of ionic reactions.

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

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

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. CH17104DCE

Title: Laboratory Course in Inorganic Chemistry (04 Credits)

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

External Exam: *75 Marks.* ***Internal Assessment****: 25 Marks*

I. Preparation of Coordination compounds of Transition metals:

1. Theoretical appraise of first row Transition metal Coordination Chemistry.
2. Synthesis as a Laboratory Technique (Concepts, Calculations and Design of Synthetic procedures).
3. Selected preparations of the following coordination compounds with the specific objectives:

i) Mercurytetrathiocyanatocobaltate(II)	:	To visualize the complexation process.
ii) Tristhioureacopper(I)sulphate monohydrate	:	Insitu generation and Stabilization of unusual oxidation state and re-crystallization /crystal growing
iii) Hexaamminecobalt(III) chloride	:	Multistep synthetic procedure
iv) Trisethylenediaminecobalt(III) chloride	:	Two stage synthesis and aerial oxidation/Resolution of a racemic mixture
v) Ammonium dodeca molbedophosphate	:	Synthesis of a heteroploy metallate/ Bonding and structure.

II. 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.

III.

A. Qualitative Analysis by Semi micro Technique:

Discussion about the analysis scheme. Analytical groups and Group reagents. Scales of Analysis, Skill of semi micro technique. Chemistry involved in separation and identification of less familiar cations by semi micro analysis.

B. Identification of four less familiar cations from different analytical groups with simple and complex combinations:

(i) Group I and II A
(ii) Group I, II A and II B
(iii) Group IIA and II B
(iv) Group I and Group III
(v) Group II B and Group III
(vi) Group III only.

IV. Inorganic Quantitative Analyses:

A. **Gravimetry:**

i) Skill and importance of weighing in Chemistry, Gravimetreric 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.

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) Barium (Ba^{2+}) as BaSO4 and Zinc as $[ZnEDTA]^{2-}$ complex.

iii) Barium (Ba^{2+}) as $BaSO_4$ and Nickel (Ni^{2+}) as $[NiEDTA]^{2-}$ complex.

iv) Nickel (Ni^{2+}) as Ni $(dmg)_2$ complex and Magnesium (Mg^{2+}) as $[Mg\ EDTA]^{2-}$ complex.

v) Copper (Cu^{2+}) as CuSCN and Magnesium (Mg^{2+}) as $[MgEDTA]^{2-}$ complex.

Books Recommended:

1. Advanced Inorganic Chemistry, 5th ed. / 6th 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; 5th edn; Jeffery, Bassett; (ELBS, 1989).
4. Quantitative Analysis; 6th edn; Day, Underwood (Printice Hall, 1993).
5. Analytical Chemistry, 6th Ed; D. Christian, Wiley.
6. Quantitative Analysis; 6th edn; Day, Underwood (Printice Hall, 1993).

Course No: CH17105DCE
Title: Symmetry and Group Theory (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

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, Symmetry groups and group multiplication tables.

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 Orthoganality Theorm-elementary idea, consequences of the Great Orthogonolity Theorem. Reducible and Irreducible representations, Mullikan symbols for IRS. Character table-construction of character tables for C2v, C3v and C4v point groups.

Applications of group theory to IR and Raman spectroscopy, 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 and Polarity.

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.

Course No: CH17106DCE
Title: Infrared, Raman and Electronic Spectroscopy (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

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_2, O_2),

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. Physical Methods for Chemists; R.S.Drago; 2nd edn; Saunders; 1992.
2. Fundamentals of Molecular Spectrsocopy; C.N.Banwell, E.M.Mc Cash; 4th edn; Tata McGrawHill; 1994.
3. Physical chemistry; P. W. Atkins; 6th edition; Oxford University Press; 1998.
4. Electronic Absorption Spectroscopy and related techniques; D N Sathyanarayna; UniversitiesPress.
5. Introductory Raman Spectroscopy; J. R. Ferraro, K. Nakamoto & C. W Brown; 2nd edn; Academic Press 2005.
6. Theory and Applications of Ultraviolet Spectroscopy; H.H.Jaffe, M.Orchin; Wiley; 1962.
7. Molecular Spectroscopy; 1st edn; J L. McHale; Prentice Hall; 1999.
8. Modern Spectroscopy; J.M.Hollas; Wiley; 1987.
9. Basic Principles of Spectroscopy; R.Chang; McGraw Hill; 1971.
10. Structural Methods in Inorganic Chemistry; 2nd edn; E.A.V.Ebsworth, D.W.H.Rankin, S.Cradock; Blackwell; 1991.

Course No: CH17001GE
Title: Chemistry of the Environment (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Soil and Hydrosphere (16 Contact hours)

Soil: Nature and Composition of soil – Air, Water, Inorganic components, organic matter and humus. Acid – Base and Ion exchange reactions in soil.

Wastes and pollutants in soil: Chemical degradation, photochemical reactions and biodegradation. Desertification, Deforestation and soil erosion.

Hydrosphere: Chemical Composition of Water Bodies: Lakes & rivers, Factors determining composition (thermal stratification, acid-base, pE concept).

Aquatic pollution: Inorganic, Organic, Pesticide, Agricultural, Industrial and Sewage.

Water quality parameters: Dissolved oxygen, Metals, Content of Chloride, Phosphate, Nitrate, and Microorganisms. Water quality standards.

Analytical Methods for determining BOD, DO, COD, and choice of methods for determining metals (As, Cd, Hg, Pb & Se).

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

Unit-II Atmosphere (16 Contact hours)

Chemical Composition of the Atmosphere: Particles, ions, radicals and their formation. Vertical profile of the atmosphere, Heat budget of earth's atmospheric system. Chemical and photochemical reactions in atmosphere, photochemical smog formation.

Oxides of N, C, S and their effects.

Ozone layer: Formation of ozone and mechanism of ozone depletion.

Pollution by chemicals: Chlorofluorocarbons, hydrocarbons and ozone.

Green house effect: Cause, source and impact on global climate.

Consequences of Green house effect and remedial measures.

Acid rain: Chemical aspects, adverse effects and control.

Books Recommended

1. Environmental Chemistry; 5th edn; Colin Baird; Freeman & Co; 2012.
2. Environmental Chemistry; 9th edn.S.E.Manahan; Lewis Publishers;2009
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 pollution; B.K.Sharma & H.Kaur; Goel Publishcrs;1996.
7. Environmental Chemistry; Nigel. J.Bunce; Wurez Publishers; 1991.
8. Environmental Toxicology; Ed.Rose; Gordon & Breach Science Publishers.

Course No: CH17002GE
Title: Surfactants and their Applications (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*

Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

Unit-I Self-Assembly of Surfactants (16 Contact hours)

***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 Systems (16 Contact hours)

a) **Mixed Surfactant systems**: Mixed micelle formation, mixed monolayer formation, synergism, various models of mixed micelle formation(Clint, Rubingh, Motamurra, Blankschtein, and Rubing-Holland models) 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. Characterization of polymer- surfactant systems by various techniques like viscosity, light scattering, spectroscopic and conductance measurements. 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. Physical Chemistry; P.W. Atkins; ELBS; Oxford; 1994.
3. Principles of Colloid and Surface Chemistry; P.C. Heimenz; Marcel Dekker Inc; New York; 1986.
4. Surfactants and Interfacial Phenomena; M. J. Rosen; John Wiley & Sons; New York; 1989.
5. Colloid and Interface Chemistry; R. D. Vold and M. J. Vold; Addison-Wesley; 1982.
6. Surfaces, Interfaces and Colloid; D. Y. Meyer; VCH Publishers; Inc; 1991.
7. Surfactants and polymers in aqueous solution; Jonsson, Lindmann, Homberg and Kronberg; John Wiley and sons; 1998.
8. Advances in Colloid and Polymer Science; B.K.Paul & S.P.Moulik, Current Science,Vol.80,p 990-,2001; Vol.78,p 99,1998.
9. Critical Reviews in Food Science and Nutrition; John Flanagan & Harjinder Singh, ,Vol. 46, pp221-237, 2006.
10. Advanced Drug Delivery Reviews; M. J. Lawrence & G.D.Rees; Vol, 45, p 898, 2000.
11. Energy Fuels; T. N. Dantas, A.A.D, Netoetal; DOI:10.1021/ ef900952y; 2010.

Course No: CH17001OE
Title: Chemistry in Everyday Life   (02 Credits)

Max. Marks: *50* | ***Duration:*** *32 Contact hours*
Ist Unit Exam: *25 marks* | ***IInd Unit (Term end) Exam:*** *25 marks*

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

(a) Water- An Amazing Chemical Stuff

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)