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.
- 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 \(\mu_s\) and \(\mu_{\text{eff}}\) values; orbital contribution to magnetic moments; applications of magnetic moment data in investigation of nature of bonding and stereochemistry of first row transition metal complexes. High spin- low spin crossover.
- 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.
10. Infrared and Raman Spectra: Inorganic and Coordination compounds ; K. Nakamoto; Wiley.
11. NMR, NQR and Mossbauer Spectroscopy 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

1st Unit Exam: 25 marks  
2nd 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.

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

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

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

Max. Marks: 100  Duration: 64 Contact hours
Ist Unit Exam: 25 marks  IIInd 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, sp² & sp³). 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-Fock self consistent field method. One and two-electron integrals in the light of minimal basis H₂ 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 Λ⁰ for weak electrolytes, Theories of Conductance: Debye-Huckel-Onsager conductance equation and brief idea of its extension.
Semiconductor electrodes: Structure of semiconductor/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 photoelectrochemistry, photoelectrochemical splitting of water, photoelectrochemical reduction of CO₂.

Books Recommended:

10. An Introduction to Aqueous Electrolyte Solutions, Margaret Robson Wright, Wiley, 2007.
Course No: CH17304DCE
Title: Laboratory Course in Physical Chemistry (04 Credits)

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

A. Conductometry
   1. Determination of the composition of a mixture of HCl and CH₃COOH 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. K₂Cr₂O₇ and determination of standard redox potential of Fe²⁺/Fe³⁺.

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 K₂Cr₂O₇ and KMnO₄ or Cobalt (II) and Nickel (II) ions.
   2. Spectrophotometric titration of Fe(II) vs. KMNO₄.

F. Chemical Kinetics
   1. Determination of order of reaction between K₂S₂O₈ and KI by Initial rates method using clock reaction.
   2. Compare the effect of ionic strength on the rate constant of persulphate-iodide reaction and iodide-Fe(III) reactions using clock method.
   3. Determination of the rate constant of inversion of cane sugar catalysed by HCl using polarimeter.

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

Max. Marks: 50  
Ist Unit Exam: 25 marks

Duration: 32 Contact hours  
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

4. Fundamentals of Analytical Chemistry; 6th Indian Reprint; D. A. Skoog and D.M. West; Cengage 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. 

Unit-II  
Applied Irreversible Thermodynamics  
(16 Contact hours)  
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 Irreversible Processes; DeGroot, Mazur; Dover; 1986.  
2. Introduction to Thermodynamics of Irreversible Processes; I. Prigogine; Wiley Interscience; 1967.  
Course No: CH17307GE  
Title: Industrial Pollution and Green Chemistry  
(02 Credits)

Max. Marks: 50  
Iso Unit Exam: 25 marks

IInd Unit (Term end) Exam: 25 marks

Duration: 32 Contact hours

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)


**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

7. Green Chemistry- An Introductory Text; IInd Edn.; Mike Lancaster; RSC; 2010.
Course No: CH17308GE  
Title: Bio-Organic Chemistry (02 Credits)

Max. Marks: 50  \hspace{1cm} Duration: 32 Contact hours
Ist Unit Exam: 25 marks  \hspace{1cm} IInd Unit (Term end) Exam: 25 marks

Unit-I  \hspace{1cm} (16 Contact hours)

(a) Chemical Origins of Biology


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.


Unit-II  \hspace{1cm} (16 contact hours)

(a) Coenzymes

Introduction, Types of coenzymes, Involvement of coenzymes in enzyme catalyzed 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
Unit-I  Representation  (08 contact hours)

Laws of nature: Knowledge, Sources 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.
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.
10. The structure of scientific revolution; Thomas S. Kuhn; The University of Chicago Press.