Course No: CH18101CR  
Title: Inorganic Chemistry (04 Credits)

Max. Marks: 100  
Duration: 64 Contact hours  
Continuous Assessment: 20 marks  
End Term Exam: 80 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 bipyramidal, octahedral and pentagonal bipyramidal molecules / ions. (PCl5, VO3-, SF6, [SiF6]2-, [PbCl6]2- and IF7). 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)


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 \(ML_6\); 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.
Preparation, reactions, structure and bonding of transition metal nitrosyls, dinitrogen and dioxygen complexes.
Tertiary phosphine as ligand.

Books Recommended
Unit-I  Delocalized Chemical bonding  (16 Contact hours)
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 \( \pi \)-electron numbers other than six (2,4,8,10 and more than ten \( \pi \)-electron systems), Aromaticity of hetero annulenes. Aromaticity in fused ring systems. Aromaticity of ferrocene and azulene. Carcinogenesis due to aromatic hydrocarbons.

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.

Unit-III  Stereochemistry:  (16 Contact hours)
Unit-IV  Aliphatic Nucleophilic Substitutions :  
(16 Contact hours)
Mechanism and stereochemical implications of $S_N2$, $S_N1$, $S_Ni$ and Neighbouring Group Participation (by $\pi$ and $\sigma$-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.


Books Recommended:

Course No: CH18103CR
Title: Physical Chemistry (04 Credits)

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

Unit-I  Quantum Chemistry (16 Contact hours)

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.

Unit-III Chemical kinetics-I (16 Contact hours)
Fast reactions: General features of fast reactions, study of fast reactions by flow method, relaxation method and flash photolysis.
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.
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 & Langmuir- Riedel mechanism], classical & statistical treatments.

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

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

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

**Books Recommended:**

Course No: CH18104CR
Title: Environmental Chemistry and Analytical Monitoring  (02 Credits)

Max. Marks: 50  Duration: 32 Contact hours
Continuous Assessment: 10 marks  End Term Exam: 40 Marks

Unit-I  Chemistry of the Environment  (16 Contact hours)
Atmosphere: Vertical profile of the atmosphere; tropospheric reactivity patterns; stratospheric chemistry (Chapman mechanism and ozone depletion).
Chemistry and control of Green house effect, Acid rain and Photochemical smog.
Hydrosphere: Factors determining composition of water bodies (acid-base, thermal-stratification, pE concept and Pourbiax diagram).
Water quality parameters: Dissolved oxygen, metals (As, Cd, Hg, Pb and Se), chloride, phosphate and nitrate. Water quality standards.
Chemistry of water treatment: Chlorination, Ozonation and UV radiation.

Unit-II  Analytical Environmental Monitoring  (16 Contact hours)
Analytical methods for measuring air pollutants: General aspects, Sampling and methods of analyses.
Continuous monitoring instruments as analytical tools for real time monitoring of air pollutants (NDIR, GC-MS, Chemiluminescence and Spectrophotometry).
Water Analysis Methods: Classical, Spectrophotometry, Electrochemical methods and Ion chromatography.
Analytical methods for determining dissolved oxygen, BOD and COD.
Choice of methods for determining trace metals (As, Cd, Hg, Pb and Se).

Books Recommended
2. Environmental Chemistry; 2nd edn; Colin Baird; Freeman & Co; 1991.
5. Environmental pollution Analysis; S. M. Khopkar; Wiley Eastern.
6. Environmental Chemistry; S. E. Manahan(6th /7th /8th /9th Edns); Lewis Publishers.

Course No. CH18105DCE
Title: Laboratory Course in Inorganic Chemistry  (04 Credits)

**Max. Marks:** 100  
**Duration:** 64 Contact hours  
**Continuous Assessment:** 20 marks  
**End Term Exam:** 80 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) Mercurytrithiocyanatocobaltate(II)  : To visualize the complexation process.
   ii) Tristhioureacopper(I)sulphate monohydrate  : In situ 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 heteropoly 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, Gravimetric Calculations
   ii) Precipitation process in homogenous mixtures, Precipitating agents, conditions of precipitation.
   iii) Precipitate processing( Digestion, Ignition); reducing precipitation errors(Co- and post precipitation)

B. Tritimetry:
   i) Types and skill of titration, concept of Complexometric titrations, tritimetric calculations.
   ii) Metallochromic Indicators: selection, structure, and mechanism of action.
   III) Role and selection of buffers in Complexometric titrations, EDTA Back titrations.

Separation and estimation of following Binary metal ion systems using Gravimetry&Tritimetry simultaneously:
   i) Silver (Ag⁺) as AgCl and Nickel (Ni²⁺) as [NiEDTA]²⁻ complex.
   ii) Barium (Ba²⁺) as BaSO₄ and Zinc as [ZnEDTA]²⁻ complex.
   iii) Barium (Ba²⁺) as BaSO₄ and Nickel (Ni²⁺) as [NiEDTA]²⁻ complex.
   iv) Nickel (Ni²⁺) as Ni (dmg)₂ complex and Magnesium (Mg²⁺) as [Mg EDTA]²⁻ complex.
   v) Copper (Cu²⁺) as CuSCN and Magnesium (Mg²⁺) as [MgEDTA]²⁻ complex.

Books Recommended:

Course No: CH18106DCE
Title: Symmetry and Group Theory (02 Credits)

Max. Marks: 50
Duration: 32 Contact hours
Continuous Assessment: 10 marks
End Term Exam: 40 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 Orthogonality 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 AB₂, AB₃, AB₄, AB₅, and AB₆ type molecules.
Applications of symmetry to Molecular Chirality and Polarity.

Books Recommended

Course No: CH18107DCE
Title: Infrared, Raman and Electronic Spectroscopy (02 Credits)

Max. Marks: 50  Duration: 32 Contact hours
Continuous Assessment: 10 marks  End Term Exam: 40 Marks

Unit-I  (a) Fundamentals of Spectroscopy  (08 Contact hours)
Interaction of light with matter, transition probability, transition moment integral, derivation of selection rules.
Natural spectral line width, broadening of spectral lines -Doppler and Collision effects.

(b) Electronic and Photoelectron Spectroscopy  (08 Contact hours)
Photoelectron Spectroscopy: Basic principles- photoionization process; ionization energies; Koopman’s theorem. Photoelectron spectra of simple molecules (N2, O2),

Unit-II  (a) Infrared Spectroscopy  (08 Contact hours)
Linear harmonic oscillator- classical and quantum treatment of vibrations, vibrational energies 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;

(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
2. Infrared and Raman Spectroscopy; Principles and Spectral Interpretation; 2nd edn.; P. Larkin; Elsevier; 2011.
5. Modern Spectroscopy; J.M.Hollas; Wiley; 2004..
Title: Surfactants and their Applications  (02 Credits)

Max. Marks: 50  
Duration: 32 Contact hours
Continuous Assessment: 10 marks  
End Term Exam: 40 Marks

Unit-I  
Self-Assembly of Surfactants  
(16 Contact hours)

**Surfactants and Micelles:** Classification of Surfactants, Solubility of Surfactants: Krafft 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

5. Colloid and Interface Chemistry; R. D. Vold and M. J. Vold; Addison-Wesley; 1982.

Course No: CH18001OE
Title: Chemistry in Everyday Life   (02 Credits)
Unit-I

(a) Water- An Amazing Chemical Stuff
Molecular structure and its unique properties. Composition of natural water.

(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
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

Books Recommended
2. Chemistry Fundamentals An Environmental Prospective; 2nd edn; Buell and Girad; Jones and Barlett; 2013.
3. www.chemistryincontext; (American Chemical Society)