Course No: CHM-201
Title: Inorganic Chemistry

Max. Marks: 100 ***Min. Qualifying Marks:*** *40%*
External Exam: *80 Marks.* ***Internal Assessment****: 20 Marks*
Total Duration: *(50 hrs.)*

Unit-I: Mechanisms of Ligand Substitution Reactions in Octahedral Metal Complexes: (12 hrs)

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.

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 metal-ligand bond breaking.

Unit-II: Mechanism of Ligand Substitution Reactions in Square-Planar complexes: (12hrs)

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-III: Electron Transfer Reactions in Coordination Complexes: (12hrs)

Complementary and non-complementary reactions. Classification as outer sphere and inner sphere redox reactions.

Mechanism of outer sphere and inner sphere electron transfer reactions:- The elementary steps involved; formation of precursor and successor complexes; rate laws. Characterization of redox reactions as outer and inner sphere.

Factors affecting the rate of electron transfer- Chemical activation; sigma and pi nature of donor/ acceptor orbitals; Electron configuration of oxidant/reductant. Bridging ligand effects in inner-sphere reactions.

Oxidative addition, reductive elimination and migration (insertion) reactions.

Unit-IV: Magnetic Properties and Electronic Spectra of Transition Metal Complexes (14 hrs)

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.

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. CHM-202
Title: Organic Chemistry

Max. Marks: 100 ***Min. Qualifying Marks:*** *40%*
External Exam: *80 Marks.* ***Internal Assessment****: 20 Marks*
Total Duration: *(50 hrs.)*

Unit-1: Aromatic Electrophilic Substitution (13 hrs)

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 reaction, 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 rearrangement and Hunsdiecker reaction.

Unit-II: Addition to carbon-hetero multiple bonds. (13hrs)

Overview of reactivity carbonyl compounds: Mechanisms of addition of water , hydrogen cyanide, alcohols , amines , organometallic reacgents 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 (12hrs)

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. (12hrs)

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 cyclo addition.

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: CHM- 203
Title: Physical Chemistry

Max. Marks: 100 ***Min. Qualifying Marks:*** *40%*
External Exam: *80 Marks.* ***Internal Assessment****: 20 Marks*
Total Duration: *(50 hrs.)*

Unit-I: Quantum Chemistry (12 hrs)

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

Angular momentum and electronic structure of atom

General theory of angular momentum. Eigen functions and Eigen values of angular momentum operators. Ladder operators. Spin angular momentum, antisymmetry and Pauli's principle. Wave functions of poly-electron atoms, Slater determinant. Atomic term symbols, term separation of pn and dn configurations, spin-orbit coupling, Zeeman splitting.

Unit-II: Surface Chemistry (13 hrs)

Liquid Surface: Surface tension, pressure difference across curved surfaces (Laplace equation), vapor pressure of droplets (Kelvin equation), Capillary condensation.

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

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

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: Solid State Chemistry-I (13 hrs)

Free electron theory of metals: The Drude Model, Lorentz modification, Sommerfield Model; Fermi-Dirac distribution function, Density of states, electron heat capacity, Hall effect.

Electron Energy Bands: Nearly free electron model, Bloch Theorem and periodicity of Bloch functions and their eigenvalues, energy bands in general periodic potential-Kronig-Penney model. Qualitative band schemes for insulators, semiconductors and metals.

Semiconductors: Intrinsic & extrinsic semiconductor (n-type & p-type). p-n junction- devices based on p-n junction (Tunnel diode, injection laser).

Unit-IV: Solid state chemistry-II (12 hrs)

Super conductors: Characteristic properties- Zero resistance, Meissner effect, Heat capacity, Thermal conductivity, absorption of em radiations and Josephson effect. BCS theory of superconductivity. 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, ELBS Oxford, 1997.*
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, Prentice Hall, 2000.*
5. *Molecular Quantum Mechanics - P. W. Atkins and R. S. Friedmann, Oxford, 1997.*
6. *Coulson's Valence, R. Mcweeny, ELBS.*
7. *Physics and Chemistry of Interfaces, H-J, Butt, K. Graf and M. Kappl, 2nd Edition, Wiley-VCH Verlag Gmbh and Co. KGaA, 2006.*
8. *Physical Chemistry of Surfaces, A. W. Adamson and A. P. Gast, 6th Edition, John Wiley and Sons, Inc. 1997.*
9. *Introduction to Solids, Azaroff, Tata McGraw,1993.*
10. *Solid State Chemistry and its Applications, West, Wiley,1989.*
11. *The Physical Chemistry of Solids, Borg, Biens, Academic press, 1992.*
12. *Solid State Reactions, Schmalzried, Academic press, 1995.*
13. *Solid State Physics, N.W.Ashcroft and N.D.Mermin, Saunders college, 2001.*
14. *Elements of Solid state Physics, J.P. Srivastava, Prentice Hall of India, 2003.*

Course No: CHM-204.
Title: Spectroscopy and Diffraction Methods.

Max. Marks: 100 ***Min. Qualifying Marks:*** *40%*
External Exam: *80 Marks.* ***Internal Assessment****: 20 Marks*
Total Duration: *(50 hrs.)*

Unit-I: Magnetic Resonance Spectroscopy (13 hrs)

Basic principles-Nuclear spin, spin angular momentum, quantization of angular momentum. nuclear magnetic moment, precessional (Larmor) frequency, energy levels in a magnetic field, resonance absorption of radio frequency radiation. Population of energy levels, Relaxation processes (T_1 , T_2).

Shielding and deshielding of magnetic nuclei. Chemical shift, its measurement and factors influencing chemical shifts; local paramagnetic and diamagnetic shielding, neighboring group anisotropy.

Spin- Spin coupling, coupling constants. Low and high resolution ^{1}H NMR spectrum of protons undergoing chemical exchange (ethanol). Chemical equivalence and magnetic equivalence. 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-II: Electron Spin Resonance spectroscopy (12 hrs)

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, Fermi contact, Spin polarization effects, Dipolar coupling, Me 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), Applications

Unit-III: Diffraction Techniques. (12 hrs)

Lattices and Unit cells; Miller indices; Laue, Bragg, and Debye-Scherrer method of X-ray structural analysis of crystals.

Indexing the reflections; identification of cubic unit cells from systematic absences in diffraction pattern.

Structure of simple lattices and X-ray intensities; structure factor and its relation to intensity and electron density; phase problem.

Introduction to neutron and electron diffraction techniques. Their comparison with X-ray diffraction technique.

Unit-IV: Chromatography and Electroanalytical methods (13 hrs)

Classification; principles – differential migration, nature of partition forces, partition coefficient, retention time, retention volume.

Plate theory, HETP, band broadening, efficiency and resolution.

Basic principles and applications of – Liquid-Solid and Liquid-Liquid column chromatography. Paper and thin layer chromatography, ion exchange (size exclusion), HPLC and Gas-Liquid chromatography. Electrophoresis.

Polarography – diffusion current, half-wave potential, Ilkovic equation, DME. (applications in organic/inorganic analysis); Amperometric titrations.

Principles of – cyclic voltametry, Anodic stripping voltametry, Coulometric titrations (Controlled current).

Books Recommended:

1. *Physical Methods for Chemists , 2nd edn. R.S.Drago (Saunders, 1992)*
2. *Fundamentals of Molecular Spectrsocopy, 4th edn- C.N.Banwell, E.M.Mc Cash (Tata McGrawHill, 1994)*
3. *Modern Spectroscopy- J.M.Hollas (Wiley, 1987)*
4. *Basic Principles of Spectroscopy- R.Chang (McGraw Hill, 1971)*
5. *Introduction to Magnetic Resonance-A Carrington, A.D.McLachlan (Harper & Row, 1967)*
6. *NMR and Chemistry, 2nd edn-J.W.Akitt (Chapman and Hall, 1983)*
7. *Theory and Applications of Ultraviolet Spectroscopy. H.H.Jaffe, M.Orchin (Wiley, 1962)*
8. *NMR, NQR, EPR, and Mossbauer Spectroscopy in Inorganic Chemistry- R. V. Parish, (Ellis Horwood,1990).*
9. *Solid State Chemistry and its Applications - West, Wiley, 1989.*
10. *Nuclear Magnetic Resonance - P. J. Hore (Oxford, 1995)*

Course No: CHM-205
Title: Chemistry of the Environment

Max. Marks: 50 ***Min. Qualifying Marks:*** *40%*
External Exam: *40 Marks.* ***Internal Assessment****: 10 Marks*
Total Duration: *(25 hrs.)*

Unit-I: Environment and Soils. (06 hrs)

Introduction , Segments of the Environment ; Factors affecting environment.

Nature and Composition of Soil : - Air, Water , Inorganic Components , Organic matter and humus. Acid Base and Ion – exchange reactions in soil.

Unit-II: Hydrosphere. (07 hrs)

Factors determining composition of water bodies :- Thermal stratification ; Acid base and redox.

PE concept :- Correlations and applications ; Pourbiax diagram (Iron & Sulphur)

Distribution diagram and oxygen sag curve.

Water Quality Parameters:- Dissolved oxygen ; Metals , content of chloride , phosphate and nitrate.

Purification & Treatment of water :- Chlorination , Ozonation and UV radiation.

Unit-III: Atmosphere. (07 hrs)

Vertical profile of Atmosphere;Heat budget of earth's atmospheric system, Atmosphere window.

Troposphere reactivity patterns ; stratospheric ozone chemistry (Chapman mechanism) and mechanism of Chlorofluorocarbon as ozone depletors.

Chemistry of Green House effect , Acid rain and Photochemical smog

Unit-IV: Analytical Methods. (05 hrs)

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

Continuous monitoring instruments as analytical tools for measuring air pollutants: NDIR, GC–MS, Chemiluminescence and Spectrophotometry.

Books Recommended:

1. *Environmental Chemistry; Nigel.J.Bunce; Wurez Publishers; 1991.*
2. *Environmental Chemistry; 2nd edn; Colin Baird; Freeman &Co; 1991.*
3. *A Textbook of Environmental Chemistry; O.D.Tyagi & M.Mehra; Anmol Publishers; 1990.*
4. *Environmental Chemistry; A.K.De; 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 Toxicology; Ed.Rose; Gordon & Breach Science Publishers.*
8. *Environmental Chemistry; S.E.Manahan; Lewis Publishers;2000*

Course No: CHM-206L
Title: Laboratory Course in Organic Chemistry

Max. Marks: 150 ***Min. Qualifying Marks:*** *40%*
External Exam: *120 Marks.* ***Internal Assessment****: 30 Marks.*
Total Duration: *(150 hrs.)*

Qualitative analyses:

Separation, Purification and identification of compounds from three component mixture (All solids). Identification on the basis of chemical tests, preparation of derivatives, Melting point comparison and IR spectroscopy.

Quantitative analyses:

- Quantitative estimation of glucose, glycine, acetone and phenols.
- Determination of iodine and saponification values of an oil sample.

Organic Synthesis:

- Acetylation of Cholesterol or salicylic acid.
- Oxidation of Cyclohexanol by chromic acid to get adipic acid.
- Aldol condensation: Dibenzal acetone and benzaldehyde.
- Cannizarro's reaction of 4-Chlorabenzaldelyde.
- Aromatic electrophillic substitutions in benzene, benzoic acid or aniline.
- Beckman rearrangement starting from acetophenone.

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)*