# CHE- 201
# INORGANIC CHEMISTRY II

**Unit-1**

**Electronic Spectral Studies of Transition Metal Complexes :** Spectroscopic ground states, correlation. Orgel and Tanabe-Sugano diagrams for transition metal complexes (d1-d9 states), Selection rule for electronic spectroscopy. Intensity of various type electronic transitions. Calculations of 10Dq, B and β parameters, charge transfer spectra.

**Unit–2**

**Magnetic Properties of Transition Metal Complexes**

Types of magnetic bodies, two sources of paramagnetism, orbital and spine effect, Curie equation and Curic-wles law, Determination of magnetic susceptibilty, Quenching of orbital contribution. Anomalous magnetic moments. Spin-Cross over and magnetic exchange coupling.

**Unit-3**

**Metal ∏ Complexes**

Metal carbonyl, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls; preparation, bonding , structure and important reaction of transition metal nitrosyl, dinitrogen and dioxygen complexes; tertiary phosphine as ligand.

**Unit-4**

**Metal Clusters**

Higher boranes, carboranes, metalloboranes and metallo-carboranes compounds dinuclear, trinuclear, tetranuclear, hexanuclear clusters with metal metal multiple bonds.

**Unit-5**

**Optical Rotatory Dispersion and Circular Dichroism**

Linearly and circularly polarized lights; optical rotatory power and circular birefringence, elipticity and circular dichroism; ORD and Cotton effect, Faraday and Kerr effects; Assignment of electronic transitions; applications of ORD and CD for the determination of (i) absolute configuration of complexes and (ii) isomerism due to non-planarity of chelate rings.

**Reference Book :-**

Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
Inorganic Chemistry, J.E. Huhey, Harpes & Row.
Chemistry of the Elements. N.N. Greenwood and A. Earnshow, Pergamon.
Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
Magnetiochemistry, R.1. Carlin, Springer Verlag.

# CHE-202
# ORGANIC CHEMISTRY II

**Unit-1**

**Aromatic Electrophilic Substitution** The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeir reactiion, Gatterman-Koch reaction .

**Aromatic Nucleophilci Substitution** The SNAr SN1, benzyne and SN1 mechanism, Reactivity effect of substrate structure, leaving group and attacking nucleophile. The Von Richte. Sommelet-Hauser, and Smiles rearrangements.

**Unit–2**

**Free Radical Reactions**

types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboyxlic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.

**Unit-3**

**Addition Reactions**

Mechanism and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio-and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bounds, hydrogenation of aromatic rings. Hydroboration, Michael reaction, sharpless asymmetric epoxidation.

**Unit-4**

**Addition to Carbon-Hetero Multiple bonds**

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acid esters and nitriles. Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and usaturated carbonyl compounds. Witting reaction. Mechanism of condensation reactions involving enolates-Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.

**Elimination Reactions**

The E2, E1 and E1 cB mechanisms and their spectrum. Orientation of the double bond. Reactitivty-effects of substrate structures, attacking base, the leavign group and the medium. Mechanism and orientation in pyrolytic elimination.

**Unit-5**

Pericyelic Reactions Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of periycyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions-conrotatory and disrotatory motions, 4n 4n+2 and ally! systems. Cycloadditions-antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotrpic reactions. Sigmatropic rearrangements-suprafacial and antarafacial

shifts of H, sigmatropic involving carbon moieties, 3,3- and 5,5 sigmatropic rearrangements. Claise n, Cope and aza-Cope rearrangements. Fluxional tautornerism, Ene reaction.

**Reference Book :-**

Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry
March, John Wiley.
Advanced Organic Chemistry, F.A. Carey and R.J. Sunderg, Plenum.
A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University Press.
Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice-Hail.
Modern Organic Reactions, H.O. House, Benjamin.
Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic 84* Professions!.

# CHE-203
# PHYSICAL CHEMISTRY II

**Unit-1**
**Chemical Dynamics**
Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory; ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions. Dyamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen-bromine and hydrogen-chlorine reactions) and homogenous catalysis, kinetics of enzyme reactions, general features fo fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis ad the nuclear magnetic resonance method, dynamics of unimolecular reactiosn (Lindemann Hinshelwood and Rice-Ramsperger-Kassel-Marcus (RRKM) theories for unimolecular reactions).

**Unit–2**
**Surface Chemistry** :-
**Adsorption** Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area (BET equation), Surface films on liquids (Electro-kinetic phenomenon).

**Micelles** Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization-phase separation and mass action models, solublization, micro emulsion, reverse micelles.

**Unit-3**
**Macromolecules:**
Polymer-definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetics of polymerization, mechanism of polymerization. Molecular mass, number and mass average molecular mass, molecular mass determination (Osmometry, viscometry, diffusion and light scattering methods), sedimentation, chain configuration of macromolecules, calculation of average dimension of various chain structures.

**Unit-4**
**Non Equilibrium Theromodynamics**
Thermodynamic criteria for non-equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g., heat flow, chemical reaction etc.) transformations of the generalized fluxes and forces, non equilibrium stationary states, phenomenological equations, microscopic reversibility and Onsager's reciprocity relations, electrokinetic phenomena, diffusion, electric conduction.

**Unit-5**
**Electrochemistry**
Electrochemistry of solutions, Debye-Huckel-Onsager treatment and its extension, ion solvent interactions. Debye-Huckel-Jerum mode. Thermodynamics of electrified interface equations. Derivation of electro capillarity, Lippmann equations (surface excess), methods of determination. Structure of electrified interfaces.
Overpotentials, exchange current density, derivation of Butler Volmer equation, Tafel plot. Quantum aspects of charge transfer at electrodes-solution interfaces, quantization of charge transfer, tunneling. Semiconductor interfaces-theory of double layer at semiconductor, electrolyte solution interfaces, structure of double layer

interfaces. Effect of light at semiconductor solution interface. Polarography theory, Ilkovic equation; half wave potential and its significance.

**Reference Book :-**

Physical Chemistry, P.W. Atkins, ELBS.

Introduction to Quantum Chemistry, A.K. Chandra, Tata Mc Graw Hill.

Quantum Chemistry, Ira N. Levine, Prentice Hall. 14. Coulson's Valence, R.Mc Ween y, ELBS.

Chemical Kinetics. K.J. Laidler, McGraw-Hill.

Kineties and Mechanism of Chemical Transformation J.Rajaraman and J. Kuriacose, Mc Millan.

Micelles, Theoretical and Applied Aspects, V. MOraoi, Plenum.

# CHE- 204
# Spectroscopy II and Diffraction Methods

**Unit-1**
**Nuclear Magnetic Resonance Spectroscopy**
Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors, influencing chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant "j" Classification (AXB, AMX, ABC, A2B2 etc.). spin decoupling; basic ideas about instrument, NMR studies of nuclei other than protin-13C, 19F and 31P. FT NMR, advantages of FT NMR.

**Unit–2**
**Nuclear Quadrupole Resonance Spectroscopy**
Quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant, splitting.
Applications.

**Unit-3**
**Electron Spin Resonance Spectroscopy**
Basic principles, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and Mc Connell relationship, measurement techniques, applications.

**Unit-4**
**X-ray Diffraction**
Bragg condition, Miller indices, Laue Method, Bragg method, Debye Scherrer method of X-ray structural analysis of crystals, index reflections, identification of 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. Description of the procedure for an X-ray structure analysis, absolute configuration of molecules.

**Unit-5**
**Electron Diffraction**
Scattering intensity vs. scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules. Low energy electron diffraction and structure of surfaces.
**Neutron Diffraction**
Scattering of neutrons by solids measurement techniques, Elucidation of structure of magnetically ordered unit cells.

# CHE- 205
# COMPUTERS FOR CHEMISTS

## This is a theory cum-laboratory co use with more emphasis on laboratory work.

**Unit-1**

**Introduction to computers and Computing** Basic structure and functioning of computer with a PC as illustrative example. Memory I/O devices. Secondary storage Computer languages. Operating systems with DOS as an example Introduction to UNIX and WINDOWS. Principles of programming Alogrithms and flow-charts.

**Unit–2**

**Computer Programming in FORTRAN/C/BASIC** (the language features are listed here with reference to FORTRAN. The instructor may choose another language such as BASIC or C the features may be replaced appropriately). Elements of the compute language. Constants and variables. Operations and symbols Expressions. Arithmetic assignment statement. Input and output Format statement. Termination statements. Branching statements as IF or GO TO statement. LOGICAL variables. Double precession variables. Subscripted variables and DIMENSION. DO statement FUNCTION AND SUBROUTINE. COMMON and DATA statement (Student learn the programming logic and these language feature by hands on experience on a personal computer from the beginning of this topic.)

**Unit-3**

**Programming in Chemistry**

Developing of small computer codes using any one of the languages FORTRAN/C/BASIC involving simple formulae in Chemistry, such as Van der Waals equation. Chemical kinetics (determination of Rate constant) Radioactive decay (Half Life and Average Life). Determination Normality, Molarity nd Molality of solutions. Evaluation Electronegativity of atom and Lattice Energy from experimental determination of molecular weight and percentage of element organic compounds using data from experimental metal representation of molecules in terms of elementary structural features such as bond lengths, bond angles.

**Unit-4**

**Use of Computer programmes**

Operation of PC. Data Processing. Running of standard Programs and Packages such as MS WORD, MS EXCEL -special -emphasis on calculations and chart formations. X-Y plot. Simpson's Numerical Integration method. Programmes with data preferably from physical chemistry laboratory.

**Unit-5**

**Internet**

Application of Internet for Chemistry with search engines, various types of files like PDF, JPG, RTF and Bitmap. Scanning, OMR, Web camera.

**Book Suggested :**

Fundamentals of Computer : V. Rajaraman (Prentice Hall)
Computers in Chemistry : K.V. Raman (Tata Mc Graw Hill)
Computer Programming in FORTRAN 1V-V Rajaraman (Prentice Hall)