

## INORGANIC CHEMISTRY-I

Subject Code	CH-HCT 1.3	IA Marks	30
No. of Lecture Hrs./Week	04	Exam Hours	03
Total No. of Lecture Hours	52	Exam Marks	70

**UNIT-I:****The Ionic bonding:****13Hrs**

Structure of ionic solids, radius ratio rules, calculation of some limiting radius ratio values coordination number 3 (planar triangle) coordination number 4 (tetrahedral) coordination number 6 (octahedral), close packing, classification of ionic structures, ionic compounds of the type AX ( ZnS, NaCl, CsCl), ionic compounds of the type AX<sub>2</sub> (CaF<sub>2</sub>, TiO<sub>2</sub>, SiO<sub>2</sub>), layer structures ( CdI<sub>2</sub>, CdCl<sub>2</sub>, NiAs).

**UNIT-II:****The covalent bond:****13Hrs**

The Lewis theory, the octet rule, sidgwick- powell theory, valence shell electron pair repulsion (VSEPR) theory, effect of lone pairs, effect of electro negativity, iso electronic principle, examples using the VSEPR theory ( Ammonia, water chlorine trifluoride, iodine heptafluoride), valence bond theory, hybridization, molecular orbital method, LCAO method (s-s, s-p, p-p, and d-d combinations of orbitals), rules for linear combination of atomic orbitals, examples of molecular orbital treatment for heteronuclear diatomic molecules(NO, CO, & HCl molecule).

**UNIT-III:****Co-ordination Compounds:****13Hrs**

Classification of coordination compounds, Werner's theory of coordination, electronic interpretation of coordination compounds, factors effecting the formation of complex ions, detection of complex ion in solution, nomenclature of coordination compounds, isomerism geometrical isomerism, optical isomerism, chelation, factors influencing the stability of metal chelates, importance of chelates, inner complexes, polynuclear complexes, theories of complex dcompounds, valence bond theory (VBT),crystal field theory(CFT),kinetic applications of crystal field theory, ligand field theory.

**UNIT-IV:****Review of Acid-Base concepts:****13Hrs**

Introduction different definitions, types of reactions, solvent system and leaving effect. A generalized acid-base concept( basicity of metal oxides hydration and hydrolysis). Measurement of acid-base strengths, steric effects (back strain, front strain and internal strain). Solvation effects with reference to liquid ammonia, anhydrous sulphuric acid, acetic acid and liquid sulphur dioxide. Hard-Soft Acids and Bases: classification, Strength of hardness and softness, Irving-William series, theoretical basis of hardness and softness.

**BOOKS RECOMMENDED:**

1. Concise inorganic chemistry - By: J. D. Lee, 5<sup>th</sup> edition Wiley India
2. Advanced Inorganic Chemistry – By: S. K. Agarwal, Keemtilal, A Pragati Edition.
3. Principles of Inorganic chemistry- By: Puri, Sharma and Pathiana, VPC (Vishal Publishing Co.)

Dept. of  
Chemistry

Chemistry

Chemistry 10/03

Employability

**FIRST SEMESTER-2019-20**

**ORGANIC CHEMISTRY-I**

Subject Code	CH-HCT 1.1	IA Marks	30
No. of Lecture Hrs./Week	04	Exam Hours	03
Total No. of Lecture Hours	52	Exam Marks	70

**UNIT-I: Stereochemistry I:**

**13Hrs**

Stereochemistry, isomerism, stereoisomerism, interconversions of projection and perspective formulae, elements of symmetry, nomenclature, molecules with one & more than one chiral centers, prostereoisomerism, resolution of racemic mixtures, racemization, stereospecific & stereoselective reaction, absolute asymmetric synthesis, optical activity in the absence of a chiral carbon & presence of chiral plane, geometrical isomerism (cis-trans), conformational analysis.

**UNIT-II: Stereo Chemistry II:**

**13Hrs**

Prochirality: Prostereoisomerism & Asymmetric synthesis Introduction, nomenclature, homotopic and heterotopic ligands and faces, Conformations and stereoisomerism of acyclic and cyclic system, conformations of cyclohexane, equatorial & axial bonds in chair form of cyclohexane, conformations of substituted cyclohexane, conformational analysis of mono & disubstituted cyclohexane, stereoisomerism of disubstituted cyclohexane, equilibria of disubstituted cyclohexane and related systems, conformations of heterocycles, polycyclic compounds, cyclohexene and cyclohexanones.

**UNIT-III: Reaction Mechanism (structure & reactivity):**

**13Hrs**

Elementary & simple reactions, transition state structure, molecularity reaction profile diagram, thermodynamics of the reaction, kinetics of the reaction, thermodynamics versus kinetic control of reactions, kinetic isotope effects, methods of determining reaction mechanisms, hard & soft acids & bases (HSAB) electrophiles & nucleophiles, reaction intermediates (carbanions, carbocations, carbon radicals, carbenes, nitrenes & benzyne)

**UNIT-IV:**

**Common name reactions:**

**13Hrs**

Michael addition, Mannich reaction, Barton reaction, Shapiro reaction, Baeyer Villiger reaction, Chichibabin reaction, Reformsky reaction, Aldol condensation reaction, Reimer Tiemann reaction, Dieckmann condensation reaction, Hofmann reaction, Schmidt reaction, S tobbe reaction, Wittig reaction, Claisen condensation reaction.

**BOOKS RECOMMENDED:**

1. Text book of physical chemistry by N.K.Vishnoi, R.J.Shukla Ane's books Pvt.Ltd. Vol I.
2. Advanced organic chemistry by Dr.Jagdamba Singh & Dr. L.D.S. Yadav, A pragati edition.
3. Stereochemistry conformation & mechanism by P.S.Kalsi.

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**PHYSICAL CHEMISTRY-I**

<b>Subject Code</b>	CH-HCT 1.2	<b>IA Marks</b>	<b>30</b>
<b>No. of Lecture Hrs./Week</b>	04	Exam Hours	03
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**UNIT-I: Solid state:**

Types of crystalline solids, space lattice (crystal lattice and unit cell), Polymorphism and isomorphism, Number of atoms/molecules/ions per unit cell, crystallography, X-ray Diffraction by crystals structure and Bragg's law, determination of crystal structure experimentally, calculations involving unit cell dimensions, structure of crystals (structure of NaCl, KCl, CsCl crystal), Imperfection in crystals (scottly defect, Frenkel defect & impurity defect).

**UNIT-II: Liquid State:****13Hrs**

Introduction, Intermolecular forces, Structure of liquids, differences between Solid, Liquid and Gases. Liquid crystals, differences between liquid crystal, solid and liquid (Phases of matter namely liquid crystal, solid and liquid), classification of liquid crystals, Structure of Nematic and cholesteric phases, Thermography, seven segment cell (Seven-segment display layout, schematic diagram).

**UNIT-III: Gaseous State:****13Hrs**

Postulates of the Kinetic theory of gases, Pressure of an Ideal gas, Gas constant (R) (Deviation from Ideal behavior of gases, causes of deviation of real gases from ideal behavior), The Van Der Waals equation of state, critical phenomenon, Continuity of states, Isotherms based on Van Der Waals equation, relation between Critical constants and Van Der Waals constants (determination of critical constants, measurements of TC, PC and critical volume VC),

**Colloidal state:**

Classifications of colloids, preparation of colloidal sols (dispersion methods, condensation methods), purification of colloidal sols, properties of colloidal sols, origin of change on colloidal sols, coagulation of colloids, protection of colloidal sols, emulsions, gels, micelle formation, CMC determination, effects of CMC, thermodynamics of CMC.

**UNIT-IV: CHEMICAL KINETICS****13Hrs**

Introduction to basic concepts, Experimental methods of following kinetics of a reaction, chemical and physical (measurement of pressure, volume, EMF, conductance, diffusion current and absorbance) methods and examples. Steady state approximation and study of reaction between NO<sub>2</sub> and F<sub>2</sub>, Kinetics of formation of HBr, HCl, decomposition of ozone, and nitrogen pentoxide. Ionic reaction: Primary and secondary salt effect.

**BOOKS RECOMMENDED:**

1. Text book of Physical chemistry – By: N.K.Vishnoi, R.T.Shukla, Ane's Book Pvt Ltd Vol I
2. Principles of Physical Chemistry- By: Puri, Sharma and Pathiana, VPC (Vishal Publishing Co.)
3. Introduction to solids – I.V.Azarrof
4. Solid state chemistry-A.R.West
5. Modern aspects of solid state chemistry – ed by C.N.Rao
6. New direction in solids state chemistry-C.N.Rao and gopal Krishanan
7. An Introduction to Electrochemistry by S. Glasstone
8. 14. Modern Electrochemistry Vol. I & II by J. O. M. Bockris and A.K.N. Reddy.
9. 15. Electrolytic Solutions by R. A. Robinson and R. H. Strokes, 1959
10. 16. Chemical Kinetics-K. J. Laidler, Pearson Education, 2004
11. 17. Kinetics and Mechanism - A. A. Frost and R. G. Pearson.
12. 18. Electrochemistry- S. Glasstone, D. Van Nostrand, 1965.

## ORGANIC CHEMISTRY-II

Subject Code	CHO HCT: 2.2	IA Marks	30
No. of Lecture Hrs./Week	04	Exam Hours	03
Total No. of Lecture Hours	52	Exam Marks	70

**UNIT 1: Heterocyclic Compounds: (14 Hrs)**

Classification, Nomenclature, Five membered heterocyclic compounds (Aromatic character, Electrophilic substitution in Furan, Pyrrole, and Thiophene), Synthesis of Furan, Pyrrole, and Thiophene, Six membered heterocyclic compounds (Pyridine; Nomenclature, preparation, Mechanism, properties and reactions), Comparison of basicity of Pyridine, Piperidine, and Pyrrole, Derivatives of Furan, Thiophene, and Pyridine, Condensed five membered and six membered heterocycles, method of synthesis and properties of Quinoline, Isoquinoline, Indole.

**UNIT 2: Synthetic Polymers: (14 Hrs)**

Classification of Polymers, Addition or chain growth polymerization, Some important Vinyl polymers (Polyethylene, Polypropylene, polyvinylchloride, polyesterene, polyvinyl acetate, Acrylonitrile, tetrafluoroethylene), Condensation or step growth polymerization (polyesters, polyamides, phenol, Urea, melamine, silicon resins, polyurathanes), Natural and Synthetic Rubber; Structure and isolation of rubber, Vulcanization, Non-Sulphur Vulcanization, polyisoprene, polyisobutylene, polybutadiene, polychloroprene, SBS, Buna-N, Environmental pollution.

**UNIT 3: (24 Hrs)****i) Aliphatic Nucleophilic Substitution:**

SN1 mechanism, SN2 mechanism, SNi mechanism, mixed SN1 & SN2 mechanism, the SET mechanism, esterification & ester hydrolysis.

**ii) Aliphatic Electrophilic Substitution:**

Unimolecular mechanism (SE1), Bimolecular mechanism (SE2 and SEi), Halogenation of aldehydes and ketones, aliphatic diazonium coupling, diazo transfer reaction.

**iii) Aromatic Electrophilic substitution:**

Nitration, Sulphonation, Halogenation, Friedel-Crafts alkylation & acylation reaction, IPSO attack, Vilsmeier-Haack reaction, Reimer-Tiemann reaction, Gatterman-Koch reaction, Fries rearrangement, Bischler-Napieralski reaction, Diazonium coupling.

**iv) Aromatic Nucleophilic substitution:**

ArSN1, ArSN2 mechanism, Aromatic nucleophilic substitution via benzyne (arynes), Sommelet Hauser rearrangement, Smiles rearrangement.

**BOOK RECOMMENDED:**

- Advanced organic chemistry by Dr. Jagdamba Singh, Dr. LDS Yadav A Pragati edition
- Text book of Organic Chemistry-Vol III - By: V.K. Ahluwalia.

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## PHYSICAL CHEMISTRY-II

<b>Subject Code</b>	<b>CHP HCT: 2.3</b>	IA Marks	30
No. of Lecture Hrs./Week	04	Exam Hours	03
Total No. of Lecture Hours	52	Exam Marks	70

**UNIT 1: Elementary Quantum Mechanics: (14 Hrs)**

Elementary Quantum Mechanics, Black body radiation, Quantum mechanics (Wien's displacement law, Stefan's Boltzmann's law), Planck's radiation law, Photoelectric effect, Bohr's model of Hydrogen atom, Compton effect, Heisenberg Uncertainty principle, Sinusoidal wave equation, Hamiltonian Operator, Schrödinger wave equation, Postulates of wave mechanics, Schrödinger wave equation for H-atom, Molecular Orbital theory, Constructions of MOs by LCAO, Physical picture of bonding and antibonding, wave functions for hybrid orbitals, comparison of MO and VB model.

**UNIT 2: Photochemistry: (14 Hrs)**

Interaction of radiation with matter, differences between thermal and photochemical processes, Laws of photochemistry, Quantum Yield, The Jablonski Diagram (Singlet and triplet excited state), Non-Radiative process, Fluorescence, Phosphorescence, Photosensitization reaction, Laser, Resonance energy transfer, New form of energy transfer process, Atomic Tug of war.

**UNIT 3: (24 Hrs)**

- i) **Electrodynamics** : Quantization of the free field: The classical theory, quantization, photons, space reflection and time reversal, causality and Uncertainty in Electrodynamics : Commutation rules, Uncertainty relations, vacuum Fluctuations : The Casimir effect, the Lamb shift, Radiative Transitions: The interaction between Field and sources, transition rates, dipole transitions, Quantum optics : The beam splitter, various states of the Field, photon coincidences, the photo effect in Hydrogen : High energies, the cross section near Threshold, scattering of photons, resonant scattering and spontaneous Decay : Model Hamiltonian, The Elastic scattering cross section, decay of the excited state
- ii) **Systems of Identical particles** : In distinguishability, second Quantization, Bose-Einstein statistics, Fermi-Dirac, the equations of motion, Distribution functions, Ideal Gas : The Grand canonical Ensemble, the Ideal Fermi Gas, the Ideal Bose gas, The mean Field Approximation: The Dilute Bose-Einstein condensate, the Hartree-Fock equations.

**BOOKS RECOMMENDED:**

1. A text book of Physical Chemistry- Vol-3-By: N. K. Vishnoi, R. J. Shukla, Ane's student edition.
2. Quantum mechanics: Fundamentals second edition by Kurt Tung-Mow Yan Springer publication.

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## ANALYTICAL CHEMISTRY-II

<b>Subject Code</b>	<b>CHA SCT: 2.41</b>	IA Marks	30
No. of Lecture Hrs./Week	04	Exam Hours	03
Total No. of Lecture Hours	52	Exam Marks	70

**UNIT 1:****(25 Hrs)**

**i) Solvent Extraction:** Principles of solvent extraction, classification of extractions, mechanism of extraction, extraction by chelation, extraction of solvating, extraction Equilibria for salvation, techniques of extraction, extraction by ion pair formation, solid phase extraction.

**ii) Supramolecules in solvent extraction:** Origin of macro cyclic and supramolecular compounds, nomenclature, classification, synthesis of Crown ethers, Cryptands and calixarenes, solvent extraction with crown ethers & cryptands, rotaxanes, synthesis of rotaxanes, metal complexes with rotaxanes, analytical application.

**UNIT 2: Electrophoresis:****(27 Hrs)**

Principles of electrophoresis, properties of charged molecules, theory of electric double layer, zone electrophoresis, isotachopheresis, isoelectric focusing, immunoelectrophoresis, techniques of electrophoresis, continuous electrophoresis, instrumentation, preparative electrophoresis, theory of capillary electrophoresis, instrumentation, sample separation, sample detections, application of capillary electrophoresis, capillary electrochromatography, miscellar electrokinetic capillary chromatography.

**BOOK RECOMMENDED:**

1. Basic concepts of analytical chemistry by S.M.Khopkar New Age International.
2. Instrumental methods of chemical Analysis, Gurudeep R Chatwal, Sharma K Anand. Himalaya publishers.

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## ORGANIC CHEMISTRY-III

<b>Subject Code</b>	<b>CHO HCT: 3.2</b>	IA Marks	30
No. of Lecture Hrs./Week	04	Exam Hours	03
Total No. of Lecture Hours	52	Exam Marks	70

### **UNIT 1: Electronic, Chiroptical and Vibration Spectroscopy: (14 Hrs)**

Considerations, Experimental methods, Beer-lamberts law. Theory and Classification of electronic transitions. Woodward Fieser rules, UV spectral study of alkenes, dienes, polymers, carbonyl & aromatic compounds. Steric effects, isobetic points, model compounds & charge transfer bands vibration spectroscopy units rotation and regions, Dispersive and FT-IR sampling techniques complimentary of IR and Raman-Fundamentals vibrations, overtones, group's frequencies, factor affecting group frequencies. Inductive resonance static effects. Mechanical coupling Fermi resonance, applications of IR in the study of H-bonding stereoisomerism, tautomerism, identification of the following organic compounds by IR, alkenes, alkynes, aromatic compounds, aldehydes, ketones, alcohol, thiols, acids amide, nitro compounds

### **UNIT 2: Proton Magnetic Resonance Spectroscopy: (24 Hrs)**

Introduction magnetic properties of nucleus, resonance condition field frequency diagram, precession of nuclei, relaxation-CW and PFT methods. Instruction & sample handling, chemical shift mechanism of shielding and deshielding in alkanes, alkenes, alkylhalides, aromatic compounds, carbonyl compounds & annulenes, chemical shifts of different types of organic compounds empirical rules spin-spin coupling geminal and vicinal coupling, relative intensities, Karplus equation curve equivalence of protons chemical & magnetic equivalence, spin-spin splitting system first order & second order patterns. Long range coupling spin decoupling (IDNP, NOE-lanthanide, shift reagents, proton attached to elements other than carbon exchange phenomena and temperature effect

### **UNIT 3: Green Chemistry: (14 Hrs)**

Introduction : Principles, Trends law, reducing market barriers, attentive feedstocks, Bergin manufacturing, designing safer chemicals, Green analytical chemistry, Green Chemistry in Practice : Yield and atom economy, the yield of a chemical reaction, reaction type and atom economy, addition, rearrangement, selectivity Supercritical Carbon Dioxide: Uses, environmental impact, the cool war, Arguments for CO<sub>2</sub>, Arguments against non-CO<sub>2</sub> refrigerants, supercritical fluid, phase diagram, natural occurrence, Venus, applications, dry cleaning, super critical fluid chromatography, chemical reactions, impregnation and dyeing, Nano and micro particle formation, super critical water oxidation, biodiesel production, supramics, carbon capture and storage, supercritical fluid deposition Catalysis: General principles of catalysis, catalysis and reduction energetics, types of catalysis, heterogeneous catalysts, Homogenous catalysts, Electro catalysts, Organocatalysis, significance of catalysis, energy processing, bulk chemicals, fine chemicals, autocatalytic reductions.

### **BOOK RECOMMENDED:**

1. Introduction to spectroscopy by D.L.Paxia, G.M.Lamman and G.S.Kriz
2. Spectroscopy of organic compounds by P.S.Kalsi
3. Text book of Green chemistry by Syed Aftab Iqbal, Neelofar Iqbal, Discovery publishing House Pvt.Ltd.

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### PHYSICAL CHEMISTRY-III

<b>Subject Code</b>	<b>CHP HCT: 3.3</b>	IA Marks	30
No. of Lecture Hrs./Week	04	Exam Hours	03
Total No. of Lecture Hours	52	Exam Marks	70

#### UNIT 1: Quantum Chemistry:

(27 Hrs)

**General principle of Quantum Mechanics:** The state of a system, quantum mechanical operators, the time dependence of wave functions, quantum mechanical operators must be Hermitian operators, A fourier series, fourier coefficient

**The Harmonic Oscillator:** A harmonic oscillator obeys Hooke's law, the energy of a Harmonic oscillator is conserved, the equation for a Harmonic oscillator model of a diatomic molecule, the harmonic oscillator accounts for the IR spectrum of a diatomic molecule, Hermite polynomials, The asymptotic solution of the harmonic oscillator, Schrödinger equation, Hermite's differential equation

**Molecules:** The Born Oppenheimer approximation, the valence bond treatment and energy of Hydrogen molecule, Heitler-London theory, the simple molecular orbital treatment of  $H_2^+$ , VBT & MO,  $Sp^2$  &  $Sp^3$  hybrid orbitals, SCF-LCAO-MO, wave functions, conjugated hydrocarbons and aromatic hydrocarbons treated by a pi-electron approximation, energies in Hückel Molecular-orbital theory, coefficients in Hückel molecular orbitals.

#### UNIT 2: Molecular Spectroscopy:

(25 Hrs)

Different regions of the electromagnetic spectrums, a rigid rotator, harmonic oscillator, rotational transitions, the intensities of the lines by a rotational Boltzmann distribution, overtones in vibrational spectra, vibration rotation interactions, vibrations of polyatomic molecules, electronic spectra, the Born Oppenheimer approximation factors, Schrödinger equation for nuclear motion, time dependent perturbation theory for selection rules, selection rule in the rigid rotator, harmonic oscillator selection rule, selection rule in electronic spectroscopy, the Franck Condon principle.

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**THIRD SEMESTER**  
**INORGANIC CHEMISTRY-III**

Subject Code	CHI HCT: 3.1	IA Marks	30
No. of Lecture Hrs./Week	04	Exam Hours	03
Total No. of Lecture Hours	52	Exam Marks	70

**UNIT-1: Photo Inorganic chemistry: (10 Hrs)**

Laws of Photochemistry, Units and Dimensions, Thermal emission and Photoluminescence, The selection Rule, Diatomic & Polyatomic molecules, The Rules Governing the transition between two energy states, Life times of excited electronic states of atoms and molecules, Two-Photon Adsorption spectroscopy, electronic, Vibrational & Rotational energies, Frank-Condon principle, Emission spectra, Wigner's spin conversion Rule, Types of photochemical pathways, Radiation less transitions, Fluorescence emission & structure, Triplet state and Phosphorescence emission, state diagrams, Delayed fluorescence.

**UNIT-2: Organometallic Chemistry: (24 Hrs)**

Definitions, Classification, Nomenclature, Characteristics, Stability of organometallic compounds, Pre-palatine Routes for metals-carbon bond formation, Group trends, Multiple bonded silicon and Arsenic organometallics, Cyclopentadienyl complexes of main group elements,  $\delta$  &  $\pi$ -bonded organometallics, organometallic compounds of Lanthanides and Actinides, Metal carbonyls  $M(CO)_y$ , Examples of Non rigid molecules in organometallic compounds, organometallic compounds as stoichiometric and catalytic Reagents, Synthesis applications of main group organometallics, Transition metal organometallics as catalytic & Synthetic reagents.

**UNIT-3: Nuclear chemistry: (18 Hrs)**

The nature of nucleus, nuclear stability, packing fraction, Magic number, Isotopes, Isobars, Isotones and Isomers, Nuclear Radioactivity, Theory of radioactivity disintegration, Radioactive equilibrium, Radioactive series, units of radioactivity, measurement of radioactivity, Nuclear Transmutation, Artificial radioactivity, Applications of radioactive Isotopes.

**BOOKS RECOMMENDED:**

- 1) Advanced Inorganic chemistry-By- S.K.Agarwal, Keentilal-A Pragati edition.
- 2) Fundamentals of Photochemistry by K.K.Rohatgi-Mukherjee
- 3) Organometallic chemistry by R.C.Mehrotra, A.Singh- New Age International 2<sup>nd</sup> addition.

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**FOURTH SEMESTER****INORGANIC SPECTROSCOPY-IV**

Subject Code	CHI HCT: 4.1	IA Marks	30
No. of Lecture Hrs./Week	04	Exam Hours	03
Total No. of Lecture Hours	52	Exam Marks	70

**UNIT 1: Mossbauer Spectroscopy:****(25 Hrs)**

Basic principle, spectral parameters, spectral display, Doppler effect, Zeeman splitting, Isomer shift, quadruple splitting, magnetic interaction, Mossbauer spectrometers, components, applications of Mossbauer techniques to the studies of bonding and structure of  $Fe^{2+}$  and  $Fe^{3+}$  compounds, detection of oxidation states

**NQR Spectroscopy:** Consequences of nuclear spin larger than  $\frac{1}{2}$  Prolate and Oblate nucleus, nuclear Quadruple charge distribution, theory and instrumentation, relations between electric field gradient and molecular structure, applications and Interaction of eQq data.

**UNIT 2: Electron Spin Resonance Spectroscopy****(27 Hrs)**

Basic principle, Zero field splitting, Kramer's degeneracy, Factor affecting g-values, Interpretation of g-values. Isotropic and anisotropic hyperfine coupling constants. Spin Hamiltonian, Spin densities and MC Connel relationship measurement techniques. ESR spin-Orbit coupling and significance of g-tensors.

**Photoelectron Spectroscopy:** Basic principles photo-electric effect, ionization process, Koopmans theorem. Photoelectron spectra of simple molecular chemical information from ESCA, Instrumentation and applications.

**BOOKS RECOMMENDED:**

1. Instrumental methods of chemical Analysis-By- Chatwal and Anand-5<sup>th</sup> edition.
2. Spectroscopy-By H. Kaur- APragati Prakashan edition.

③ Bioinorganic chemistry

④ Metal-ligand equilibria in solution

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## PHYSICAL CHEMISTRY-IV

<b>Subject Code</b>	<b>CHP HCT: 4.3</b>	IA Marks	30
No. of Lecture Hrs./Week	04	Exam Hours	03
Total No. of Lecture Hours	52	Exam Marks	70

### UNIT 1: Chemical Kinetics and Catalysis

(25 Hrs)

Introduction, rate of chemical reaction, factors influencing the rate of reaction, concentration dependence of reaction rate, molecularity and order of reaction, zero order reactions, first order reactions, pseudo unimolecular reaction, second order and third order reactions, radio decay as a first order phenomenon (radio-dating, Mineral dating, carbon dating), determination of order of reactions (differential, integration, half life and isolation method), experimental methods of chemical kinetics (conductometric titrations, potentiometric measurements, optical methods and spectrophotometric method), theories of chemical kinetics (simple collision theory based on Hard Sphere Model, transition state theory, thermodynamic treatment of transition state theory), complex reactions, catalysis: characteristics of catalyzed reactions, classification of catalysis, miscellaneous examples: Monsanto process for the production of Acetic acid, Ziegler-Natta catalyst, Hoechst-Wacker process, Heck Reaction.

### UNIT 2: Chemical Thermodynamics:

(27 Hrs)

- i) **The first law of Thermodynamics:** The law of conservation of Energy, Physical significance of  $E$ , Work done in a System, Heat change at constant Volume ( $q_v$ ) and constant pressure ( $q_p$ ), Heat capacity, Variation of internal energy with temperature and volume, Enthalpy as a function of 'T' and 'P', Joule-Thomson porous plug experiment, reaction between  $C_v$  and  $C_p$ , Real gases: Non-Ideal gases.
- ii) **Thermochemistry:** Thermochemical equations, Laws of thermochemistry, Born-Haber Cycle, Bond energies, Variation of heats of relation with temperature and with pressure.
- iii) **The second law of Thermodynamics:** Relevance of the second law, The concept of Entropy, Combined form of first and second law of thermodynamics, Entropy change for isolated system, Calculation of entropy changes, Third law of thermodynamics and evaluation of absolute entropy, Entropy at equilibrium.
- iv) **Free energy functions and Statistical thermodynamics:** Purpose of new functions, Properties of Helmholtz free energy and Gibbs free energy, Thermodynamic equilibrium and free energy functions, Coupled reactions, Physical equilibria involving phase transitions, entropy of vaporization, and Trouton's Rule. Quantum mechanical aspects; The rule of statistical mechanics, Probability and entropy, The Boltzman Distribution law, The partition function, Partition function of polyatomic molecules, Translation partition function, Rotational partition function, Vibrational and Electronic partition function.

### BOOKS RECOMMENDED:

1. Text book of Physical chemistry -By: N.K. Vishnoi, R.J. Shukla.
2. An introduction to Chemical Thermodynamics -By: R.R. Rastogi R.R. Mishra.

③ Molecular Spectroscopy  
 ④ Polymer Science & Technology

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## 4.2 ORGANIC CHEMISTRY-IV

Subject Code	CHO HCT:	IA Marks	30
No. of Lecture Hrs./Week	04	Exam Hours	03
Total No. of Lecture Hours	52	Exam Marks	70

### UNIT-I Multi-Nuclear NMR and Correlation Spectroscopy: (25 Hrs)

<sup>13</sup>C-NMR broad band and off resonance decoupling methods of detection, <sup>13</sup>C-chemical shift of different classes of organic compounds, alkyl halides, alkenes, alcohols, ethers and aromatic compounds, <sup>13</sup>C-H coupling DEPT, introductory aspects of <sup>15</sup>N, <sup>19</sup>F, <sup>31</sup>P-NMR, correlation NMR spectroscopy

**Mass spectroscopy: I) Ionization and mass analysis:** Instrumentation, methods of ionization EI, CI, DI, SI-methods.

**II) Fragmentation Principle,** odd and even electron ions, molecular ion and base peak, nitrogen rule, metastable ions, isotopic effect in chloro and bromo compounds, Sterenson rule.

**III) Fragmentation of** Normal and branched alkanes, alkenes, benzene & its derivatives, alcohols, aldehydes, ketones, acids, esters, ethers, amines, nitro compounds, halo compounds, calculation of molecular formula, composite problems.

### UNIT 2: Pericyclic reactions: (27 Hrs)

Introduction, symmetry in linear conjugated pi-systems symmetry in allyl and 2,4-pentadienyl systems, types of pericyclic reactions, electrocyclic reactions: FMO method, cyclisation of (4n+2)π system, Hückel-Mobius (4n) method, cycloaddition reactions, FMO method: (2+2) and (4+2) cycloaddition reactions, Hückel -Mobius method, 1,3-dipolar cycloadditions, chelotropic reactions, sigmatropic rearrangement, analysis of sigmatropic rearrangement by FMO method, Claisen rearrangement, Hückel-mobius method in sigma tropic rearrangements, group transfer reactions : Ene reactions

### Books recommended:

1. Spectroscopy of organic compounds by P. S. Kalsi
2. Advanced organic chemistry by Dr. Jagadamba Singh, Dr. L. D. S. Yadav 4<sup>th</sup> edition a pragati edition.

*Oxidation reactions*  
*Chemistry of heterocyclics*