# COURSES OF STUDY M.Sc. (CHEMISTRY)



SCHOOL OF CHEMISTRY (AUTONOMUS) SAMBALPUR UNIVERSITY Jyoti Vihar, Burla - 768 019

# M. Sc. SEMESTER SYLLABUS

	COURSE TITLE	CREDITS
NO	1 <sup>st</sup> SEMESTER	
CHI-401	GROUP THEORY, SOLID STATE & NUCLEAR CHEMISTRY	3
CHI-402	TRANSITION METAL CHEMISTRY	3
CHO-403	STRUCTURE AND REACTIVITY	3
CHO-404	STEREOCHEMISTRY	3
CHP-405	THERMODYNAMICS	3
CHP-406	DYNAMICS	3
CHI-407	INORGANIC GENERAL PRACTICAL-I	2
CHO-408	ORGANIC GENERAL PRACTICAL-I	2
	TOTAL	22

# 2<sup>nd</sup> SEMESTER

CHO-418	ORGANIC GENERAL PRACTICAL-II	2
CHI-417	INORGANIC GENERAL PRACTICAL-II	2
CHP-416	SURFACE CHEMISTRY	3
CHP-415	QUANTUM CHEMISTRY	3
CHO-414	ORGANIC REACTION MECHANISM - II	3
CHO-413	ORGANIC REACTION MECHANISM - I	3
CHI-412	BIO-INORGANIC CHEMISTRY	3
CHI-411	METAL $\pi$ -COMPLEXES AND CLUSTERS	3

TOTAL 22

### **3rd SEMESTER**

		TOTAL	24
	EXTRA DEPARTMENTAL COURSE		2
CHP-508	PHYSICAL GENERAL PRACTICAL-II		2
CHP-507	PHYSICAL GENERAL PRACTICAL-I		2
CHP-506	SPECTROSCOPY-I		3
CHP-505	STATISTICAL MECHANICS		3
CHO-504	PERICYCLIC REACTION, PHOTOCHEMISTRY & REAGENTS		3
CHO-503	NATURAL PRODUCTS & SPECTROSCOPY		3
CHI-502	INORGANIC REACTION DYNAMICS		3
CHI-501	INSTRUMENTAL METHODS OF ANALYSIS		3

# 4<sup>th</sup> SEMESTER

**Elective Courses:** A student will choose two theory elective courses and two practical courses from one branch only.

	2 Elective Courses		06
CHG-551	BIOMOLECULES		03
CHG-552	SPECTROSCOPY-II		03
CHC-553	COMPUTER APPLICATION IN CHEMISTRY		02
CHC-554	PRACTICAL ON COMPUTER IN CHEMISTRY		02
CHG-555	SYNTHETIC PRACTICAL		02
CHG-556	ANALYTICAL PRACTICAL		02
CHR-557	REVIEW WORK		02
CHS-558	SEMINAR		02
		TOTAL	24
	INORGANIC CHEMISTRY (Elective)		
CHI-511	ORGANOMETALLIC CHEMISTRY		03
CHI-512	ANALYTICAL CHEMISTRY		03
	ORGANIC CHEMISTRY (Elective)		
CHO-521	ORGANIC SYNTHESIS - I		03
CHO-522	ORGANIC SYNTHESIS - II		03
	PHYSICAL CHEMISTRY (Elective)		
CHP-531	PHOTOPHYSICAL CHEMISTRY		03
CHP-532	POLYMER CHEMISTRY		03
	INDUSTRIAL CHEMISTRY (Elective)		
CHIn-541	MATERIAL AND ENERGY BALANCE		03
CHIn-542	INDUSTRIAL PROCESSES		03

### **FIRST SEMESER**

### CHI-401: GROUP THEORY, SOLID STATE & NUCLEAR CHEMISTRY

3 credits

UNIT-I: GROUP THEORY

Symmetry elements and symmetry operation. Matrix representation of symmetry operation. Groups, subgroup, classes and group multiplication table. Point groups and their deduction by flow chart method, Study of C<sub>n</sub>, C<sub>n</sub>, C<sub>n</sub>, D<sub>n</sub>, D<sub>n</sub>, D<sub>n</sub>, D<sub>n</sub>, D<sub>n</sub>, D<sub>o</sub>, D<sub>o</sub>,

#### UNIT-II: SOLID STATE CHEMISTRY

- (a) Crystal lattice, Crystal planes, Miller indices, Bragg's law, Determination of crystal structure (NaCI, KCI), Structure of elements and compounds.
- (b) Bonding in Solids: Van der waal's force, force of covalency, bonding in ionic solids, Born-Harber cycle, theoretical evaluation of lattice energy, imperfections in solids, Schottky and Frenkel defects.

#### UNIT-III: NUCLEAR CHEMISTRY

- General characteristics of radioactive decay, Decay kinetics, Parent-daughter decay growth relationship, α-decay, β-decay & γ-emission.
- (b) Nuclear fission, Process of nuclear fission, Fission fragments and their mass distribution, Charge distribution, Ionic charge of fission fragments, Fission energy, Fission cross-sections and thresholds, Fission neutrons, Theory of nuclear fission. Fission.

#### BOOKS: Unit-I : Group Theory by F.A.Cotton Unit-II : Solid State Chemistry by D.K.Chakravarty. Unit-III: Nuclear Chemistry by J.Arniker.

#### CHI-402: TRANSTION METAL CHEMISTRY

UNIT-I

THEORIES OF METAL-LIGAND BONDING

- a. Crystal field theory (CFT): Splitting of d-orbital under the influence of octahedral, tetrahedral, tetragonal, square planar, trigonal bipyramidal and square pyramidal fields, Streochemical and thermodynamic effect of CF splitting, CFSE and Jahn-Teller effect.
- b. Molecular orbital theory (MOT): Sigma bonding in octahedral complexes: Classification of metal valence orbitals into sigma symmetry, formation of ligand group orbitals (LGOs) of sigma symmetry, Formation of molecular orbitals of sigma symmetry, construction of molecular orbital energy level diagram involving only sigma bond contribution from ligands, pi bonding in octahedral complexes, Classification of metal valence orbital into pi symmetry, Formation of LGOs of pi symmetry. Formation of pi MOs and construction of molecular orbital energy level diagram involving sigma and pi contribution from pi donor ligands, Sigma and pi bonding in tetrahedral complexes.
- c. Ligand field theory (LFT) and adjusted crystal field theory (ACFT).

#### UNIT-II

#### COMPLEX EQUILIBRIA AND TERM DIAGRAM

- a. Complex Equilibria: Types of complex equilibria in solution and types of complex equilibrium constant (stability constant), The complex formation functions, Determination of stability constant by spectrophotometric method and pH titration method, Stabilization of unusual oxidation state.
- b. Term Diagram: Russell-Saunders or L-S coupling scheme, Term symbols and their derivation by Pigeon-Hole diagram especially for p<sup>n</sup> and d<sup>n</sup> configuration, Inter-electron repulsion parameters and spin-orbit coupling parameters, The effect of weak crystal field on S, P, D, F, G, H and I terms, Orgel diagram for d<sup>1</sup> to d<sup>9</sup> configuration, Term interaction and the energies of the levels.
- c. Correlation diagram: Strong field configuration of O<sub>h</sub> symmetry, the method of descending symmetry, correlation diagram for d<sup>2</sup> and d<sup>3</sup>confuguration, Tanabe-Sugano diagram(qualitative explanation and significance).

#### 3 Credits

### M. Sc. Courses of Study

#### UNIT-III ELECTRONIC SPRCTRAL AND MAGNETIC PROPERTIES OF METAL COMPLEXS

- a. Electronic spectral properties of metal complexes: Introduction, types of experimental recording of the spectra, selection rules (mechanism of electronic transition, orbital selection rule, Laporte rule or purity selection rules, spin selection rule), Relaxation of selection rules (departure from cubic symmetry d-p mixing vibronic coupling), Nature of electronic spectral bands with respect to band intensity and bandwidth, Classification of electronic spectra. Ligand field spectra of octahedral and tetrahedral complexes and evaluation of Dq, B' and beta(β) parameters for the complex with T<sub>1</sub> ground state and A<sub>2</sub> ground state, Spectrochemical and nephlelauxetic series, charge transfer spectra.
- b. Magnetic properties of metal complexes: Origin of magnetic behavior, concept of magnetic susceptibility, dia, para, ferro and antiferro magnetism, magnetic moments from multiple width cases, quenching of orbital magnetic moment by crystal field, spin-orbit coupling and anomalies magnetic moments, Spin-crossover in coordination compounds.
- **BOOKS:** 1. Theoretical Inorganic Chemistry : M. C. Day and J. Selbin
  - 2. Advanced Inorganic Chemistry : F. A. Cotton and G. Wilkinson
    - 3. Introduction to Ligand Field : B. N. Figgs

#### CHO-403: STRUCTURE AND REACTIVITY

3 credits

#### UNIT-I: NATURE OF BONDING IN ORGANIC MOLECULES

Delocalized chemical bonding, Conjugation, Cross conjugation, Resonance, Hyperconjugation, Bonding in fullerenes, Tautomerism. Aromaticity in benzenoid and non-benzenoid compounds, Alternant and non-alternant hydrocarbons, Huckel's rule, energy levels of pi-molecular orbitals of simple systems, Annulenes, Anti-aromaticity, Homo-aromaticity, Bonds weaker than covalentaddition compounds, Crown ether complexes and cryptands, Inclusion compounds, Cyclodextrins, catenanes and rotaxanes.

#### UNIT-II: REACTION MECHANISM: STRUCTURE AND REACTIVITY

Types of mechanisms, Types of reactions, Thermodynamic and kinetic requirements, Kinetic and thermodynamic control, Hammond's postulate, Potential energy diagrams, Transition states and intermediates, Methods of determining mechanisms, Hard and soft acids and bases, Effect of structure on reactivity: Resonance and field effects, Steric effect, Quantitative treatment, The Hammett equation and linear free energy relationship, Substituent and reaction constants, Taft equation.

#### UNIT-III:

(a) REACTION INTERMEDIATE

Non-classical carbocations, Free radicals, Carbenes, Nitrenes, Arynes.

(b) GENERAL DISCUSSION ON THE FOLLOWING

Solvent effect, Isotope effect, Kinetic salt effect, Stereoselective, Regioselective, Stereospecific and Regiospecific reactions, Stereo electronic factors in transition state stability.

- BOOKS:
   1. Advanced Organic Chemistry: Reaction Mechanism and Structure Jerry March (Wiley Eastern Limited)

   2. Physical basis of organic chemistry (Wiley Eastern Limited).
   N. Isaac
  - Mechanism and theory in organic chemistry (Harper Row Lowry and Publishers, New York)
     Organic Chemistry
     Morrison and Boyd

### M. Sc. Courses of Study

#### CHO-404: STEREOCHEMISTRY

- *UNIT-I:* Chirality, Fischer projection and R and S notations, Threo and erythro nomenclature, E and Z nomenclature, Optical isomerism in biphenyls and allenes, Concept of Prostereoisomerism and Assymetric synthesis (including enzymatic and catalytic nexus), Conformation of a few acyclic molecules (alkanes, haloalkanes), Conformation of cyclic systems having one and two sp2 carbon atoms.
- UNIT-II: Dynamic stereochemistry: Conformation and reactivity, Selection of substrates, Quantitative correlation between conformation and reactivity, (Weinstein-Eliel equations and Curtin-Hammett principles), Conformational effects on stability and reactivity in acyclic compounds (ionic elimination, intramolecular rearrangements, NGP) and in cyclic systems, (Nucleophilic substitution reaction at ring carbon, Formation and Cleavage of epoxide rings, Addition reactions to double bonds, Elimination reactions).
- *UNIT-III:* Molecular dissymmetry and chiroptical properties, Linearly and circularly polarised lights, Circular birefringence and circular dicroism, ORD, Plane curves, Cotton effect, Rotatory Dispersion of ketones, Axial haloketone rule, the Octane rule. Helicity rule, Lowe's rule, Emperical rule involving the benzene chromophore.

#### BOOKS:

1.	Stereochemistry of organic compounds	: D. Nashipuri.
2.	Stereochemistry	: Kalsi
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3. Stereochemistry : Elliel

#### CHP-405: THERMODYNAMICS

#### UNIT-I: CLASSICAL THERMODYNAMICS

Brief resume of the concepts of laws of thermodynamics, Free energy, chemical potential and entropy, Third law of thermodynamics and determination of entropy, Entropy and probability, Boltzmann-Planck equation, Partial molar properties (partial free energy, molar volume and molar heat content), Their significance and determination. Concept of fugacity and its determination.

#### UNIT-II THERMODYNAMICS OF LIVING SYSTEMS Bioenergetics and thermodynamics, Phosphate group transfer and ATP, Biological oxidationreduction reactions.

#### UNIT-III NON-EQUILIBRIUM THERMODYNAMICS Microscopic reversibility, Entropy productions and irreversible process, Different types of forces and fluxes, Steady states & Cross phenomena, Phenomenological equations, Onsager reciprocity theorem, Chemical Reactions.

#### CHP-406: DYNAMICS

UNIT-I: CHEMICAL KINETICS

Theories of reaction rates, Collision theory, Transition state theory, Arrehenius equation and the activated complex theory, Reaction between ions, Salt effect, Steady-State Kinetics, Kinetic and Thermodynamic concept of Reactions, Treatment of unimolecular reaction (Lindemann-Hinshelwood and Rice-Ramspeger-Kassel-Marcus (RRKM) theories), Dynamic chain ( $H_2 + Br_2$  reaction, pyrolysis of CH<sub>3</sub>CHO, Decomposition of ethane).

#### UNIT-II: CATALYTIC & FAST REACTION Kinetics of Catalytic Reactions: Acid-base Catalysis, Enzyme Catalysis, Heterogeneous Catalysis. Fast reactions: General feature, Study of Fast reactions by relaxation, Stopped flow and Flash photolysis.

#### UNIT-III: ELECTROCHEMISTRY

Interionic attraction theory and Debye-Huckel treatment, Derivation of Onsager limiting law and its verification and modification, Activities, activity coefficients, Debye-Huckel treatment, Debye-Huckel-Bronsted equation, Salt effect, Determination of activity coefficients from solubility method, lon association, Determination of thermodynamic dissociation constant of weak electrolytes by Shedlovsky method and by EMF method, Nernst equation, redox systems, electrochemical cells.

### 3 Credits

3 Credits

6.

7.

#### BOOKS:

- 1. Text Book of Physical Chemistry Vol-1-4: K.L. Kapoor
  - 2. Physical Chemistry 3. Principles of Physical Chemistry

4. Physical Chemistry

10. Electrochemistry

12. Chemical Kinetics

13. Reaction Kinetics

Chemical Thermodynamics

8. Molecular Thermodynamics

9. Principle of Biochemistry

Thermodynamics for Chemists

11. Modern Electrochemistry Volume-I

- : D.N. Bajpai : Puri, Sharma & Pathania
- : A.W. Atkins
- 5. Physical Chemistry Through Problems : Dogra & Dogra
  - : Rastogi & Mishra
  - : S. Glasstone

    - : McQuarrir & Simon
    - : A.L. Lehninger
    - : S. Glasstone
    - : Bookris & Reddy : K.J. Laidler
  - : Pilling & Seakins

#### CHI-407: **INORGANIC GENERAL PRACTICAL-I**

Analysis of an inorganic mixture containing not more than 6 radicals. The mixture will include rare earth like Tungstate, Vanadate, Molybdate and Cerium (IV). Insoluble matters and other interfering radicals will also be included. Organic radicals are excluded.

#### CHO-408: **ORGANIC GENERAL PRACTICAL-I**

Isolation and identification of multi-functional compounds in a mixture of two organic compounds.

2 Credits

2 Credits

### SECOND SEMESTER

#### CHI-411: METAL π-COMPLEXES AND CLUSTERS

3 credits

#### UNIT-I CARBON MONOOXIDE COMPLEXES

Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reaction of metal carbonyls, carbonylate anions and carbonylate hydride, carbonyl halides and related compounds. Nature of M-C bond in carbonyls.

#### UNIT-II COMPLEX OF CARBON MONOXIDE ANALOGS

- (a) Preparation, bonding and important reaction of transition metal complexes with isocyanide, cyanide, dinitrogen, carbon disulphide and nitrogen monoxides.
- (b) Transition metal to carbon multiple bonded: compounds chemistry of carbenes, carbynes.

#### UNIT-III METAL CLUSTER AND POLYACIDS

- (a) Metal cluster: Occurrence of metal-metal bonds in metal complexes, Bonding in metal cluster. Metal carbonyl type clusters. Anionic and hydride cluster. Method of synthesis, super large cluster, electron counting in medium size cluster (Wade's rule, Capping rule), Isolable relationship, cluster of Fe, Ru, Os groups. Cluster of Co, Rh, Ir groups. Cluster of Ni, Pd, Pt groups. Catalysis by cluster.
- (b) Isopoly and heteroply acids and salts.
- **BOOKS:** 1. Advance Inorganic Chemistry: F.A. Cotton, G. Wilkinson & C. Murillo (6<sup>th</sup> edition).
  - 2. Inorganic Chemistry: J.E. Helay, Harper and Row
  - 3. Comprehensive Coordination Chemistry : Eds. Wilkinson, Gillarsand
  - 4. Modern Aspect of Inorganic Chemistry :Emelius and Sharpe

#### CHI-412: BIO-INORGANIC CHEMISTRY

3 credits

#### UNIT-I TRANSPORT AND STORAGE OF METALS

Metal ions in biology with special reference to Na , K, Mg, Ca, Fe, Zn, Co and Mo, The transport mechanism, Transport and storage of alkali and alkaline earth metal, Transport by neutral macrocycle, Transport by anionic carriers, sodium/potassium pump, calcium pump, ionophores and their role as ion carrier, transport and storage of iron, Ferritin, transferrin(siderophilin), siderophores, Storage of copper and zinc, metello thioneines, transport of copper and zinc.

#### UNIT-II METALLOPORPHYRINS AND IRON-SULPHUR PROTEIN

- a. Iron porphyrins (Heme proteins): Hemoglobin (Hb), Myoglobine (Mb) their behavior as oxygen carrier and oxygen uptake protein, O<sub>2</sub> affinity cooperativity and Bohr's effect, Heme protein as electron carrier with particular reference to reference to cytochrome-c and cytochrome-450, and cytochrome oxydase.
- b. Magnesium porphyrins (Chlorophyll): Photosynthesis, the light and dark reaction (Calvin cycle).
- c. Non-heme iron-sulphur protein as electron carrier, rubredoxins and ferredoxins.

#### UNIT-III METALLOENZYMES

Preliminary idea about enzyme, co-enzyme and metalloenzyme, Enzyme-substrate binding problem, The Michaelis-Menten's equation, carboxypeptidase, carbonic anhydrase and their biological significance, oxydases, nitrogenases and its role in nitrogen fixation, Interchangeability of zinc and cobalt enzyme

BOOKS:	1.	Basic Inorganic Chemistry (3 <sup>rd</sup> ed)	: Cotton ,Wilkinson & Gaus
	2.	Inorganic chemistry (4 <sup>th</sup> Ed)	: Huheey, Keiter & Keiter
	3.	Bioinorganic and Suparmolecular Ch	emistry: Bhagi,G.R.Chatwal
	4.	Bio-Inorganic chemistry	: E.Ochiai

- Bio-Inorganic chemistry
   Bio-Inorganic chemistry
- : R.W.Hay

#### CHO-413: **ORGANIC REACTION MECHANISM - I**

3 credits

- UNIT-I The  $S_N2$ ,  $S_N1$ , mixed  $S_N1$  and  $S_N2$  and SET mechanisms. The neighbouring group mechanism, Neighboring group participations by sigma and pi bonds, anchimeric assistance. Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements, application of NMR spectroscopy in the detection of carbocations. The S<sub>N</sub>I mechanism. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis, ambident nucleophile, regioselectivity.
- Alipahatic Electrophilic Substitution mechanism: S<sub>E</sub>1, S<sub>E</sub>2 and S<sub>E</sub><sup>1</sup> mechanisms, Effect of UNIT-II a. substrate, leaving group and solvent, Reactions (hydrogen exchange, migration of double bonds, keto-enol tautomerism, halogenation, aliphatic diazonium coupling, Stork-enamine reaction).
  - Aromatic electrophilic substitution mechanism: Structure reactivity relationship in monoh substituted benzene, ring isomer proportions, orientation in benzene ring with one or more than one substituent, Orientation in other ring systems, Vilsmeir - Haack reaction, Pechmann reaction.
- UNIT-III Aromatic Nucleophilic Substitution mechanism: Introduction, to different mechanisms, а. Aromatic nucleophilic substitutions ( $S_NAr$ ,  $S_N1$  aryne), Effect of substrates, leaving groups, and nucleophile, Reactions: Nucleophilic displacement in areno-diazonium salts by different nucleophiles, Chichibabin reaction.
  - b Free radical Substitution: Reaction at sp<sup>2</sup> carbon, Reactivity in aliphatic substrates, Reactivity at bridge head position, Reactivity in aromatic substrates.
- BOOKS: 1. Advanced Organic Chemistry: Reaction Mechanism and Structure (Willey Jerry Eastern Limited) March
  - **Organic Reaction Mechanism** 2.

#### CHO-414: **ORGANIC REACTION MECHANISM - II**

- UNIT-I
- Addition to carbon-carbon multiple bonds, Electrophilic, Nucleophilic and Free radical a. addition, Orientation and Reactivity, Addition to cyclopropanes, Reactions: Hydroboration, Michael reaction, Sharpless Asymmetric epoxidation.
  - b. Addition to carbon-heteroatom multiple bonds: Mechanism and reactivity, Reactions: Mannich reaction, LiAlH<sub>4</sub> reduction of carbonyl compounds, acids, esters, nitriles, addition of Grignard reagents - Reformatsky reaction, Aldol condensation, Knoevenagel condensation, Perkin reaction, Tollens reaction, Wittig reaction, Prins reaction, Benzoin condensation.
- UNIT-II Elimination mechanism: E<sub>1</sub>, E<sub>2</sub>, E<sub>1</sub>CB and E<sub>2</sub>CB mechanisms, Orientation, Effect of substrate, base, leaving group and medium, Orientation of double bond, Sayetzeff and Hoffman rules, Pyrolytic elimination reaction, Oxidative elimination (oxidaton of alcohol by chromium, Moffatt oxidation). Reactions: Cleavage of quaternary ammonium hydroxides, Chugaev reaction, Shapiro reaction.

#### UNIT-III REARRANGEMENTS

General mechanistic considerations - nature of migration, migratory aptitude, memory effects.

A detailed study of the following rearrangements, Wagner-Meerwein, Favorskii, Arndt-Eistert synthesis, Neber, Beckmann, Hofmann, Schmidt, Lossen, Curtius, Baeyer-Villiger, Shapiro reaction, Von-Ritcher, Sommelet-Hauser rearrangement.

BOOKS:	1. Advanced Organic Chemistry: Reaction Mechanism and Structure (Willey	Jerry
	Eastern Limited)	March
	2. Organic Reaction Mechanism	Kalsi
	3. Physical Basis of Organic Chemistry (Wiley Eastern Limited)	N. Isaac

3. Physical Basis of Organic Chemistry (Wiley Eastern Limited)

3 credits

Kalsi

#### CHP-415: QUANTUM CHEMISTRY

#### UNIT-I EXACT QUANTUM MECHANICAL RESULTS

The Schrodinger equation and the postulates of guantum mechanics, Elementary application of the Schrodinger equation, Particle in a box, Harmonic oscillators, Rigid rotator and hydrogen atom.

#### UNIT-II APPROXIMATE METHODS & ANGULAR MOMENTUM

The variation theorem, Time independent perturbation of non-degenerate systems, Application of Variation Method and Perturbation Theory to the He atom. Ordinary angular momentum, generalized angular momentum, Eigen functions for angular momentum, Addition of angular momentum.

#### UNIT-III HUCKEL MOLECULAR ORBITAL THEORY

Huckel theory of conjugated systems (Ethylene, Allyl systems, butadiene, cyclopropenyl, cyclobutadiene, bicyclobutadiene,  $H_3^+$ ,  $H_3$  and  $H_3^-$ ), Calculation of bond order, charge density, free valence index, Application of group theory for the simplification of MO determinants of 1.4- butadiene and naphthalene.

#### CHP-416: SURFACE CHEMISTRY

#### PHASE RULE UNIT-I

Concept of Equilibrium between phases, Derivation of phase rule, Ideal Solution, Liver Rule, Brief concept on one and two component system, Application of phase rule to three component systems of both solids and liquids.

#### UNIT-II ADSORPTION

Surface tension, Capillary action, Adsorption, types of adsorption, Gibbs adsorption isotherm, Freundlich's adsorption isotherm, Langmuir's adsorption isotherm and its limitations, BET adsorption isotherm and its applications, Heat of adsorption, estimation of surface areas of solids from solution adsorption studies, Brief concepts on micelle, reversed micelle and microemulsions.

#### UNIT-III MACROMOLECULES

Polymer-definition, Types of polymer, Number average and weight average macromolecules, determination of molecular weights of macromolecules (Osmometry, Viscometry, Diffusion and Light scattering method), Kinetics of polymerization, Donnan Effect, Stereochemistry of polymerization.

#### BOOKS: Text Book of Physical Chemistry Vol-1-4: K.L. Kapoor 1.

- 2. Physical Chemistry
- : D.N. Baipai : Puri. Sharma & Pathania : A.W. Atkins
- 3. Principles of Physical Chemistry 4 Physical Chemistry
- 5. Physical Chemistry Through Problems : Dogra & Dogra : A.K. Chandra
- Introductory Quantum Chemistry 6.
- 7. Notes on Molecular Orbital Calculations : J.D. Roberts : R.K. Prasad
- 8. Quantum Chemistry Polymer Science 9.
- : Gowariker, Viswanathan & Sreedhar

#### **INORGANIC GENERAL PRACTICAL-II** CHI-417:

- 1. Principle of estimation of the main constituents of Brass and Portland Cement.
  - (a) Estimation of Ca and Mq in a given solution prepared from a sample of cement by EDTA method .
  - (b) Estimation of Cu and Zn in a given solution prepared from a sample of Brass.
- Determination of MnO<sub>2</sub> in pyrolusite. 2
- Preparation and cheracterisation of the following inorganic compounds: 3
  - (i) Tetramminecupric sulphate [Cu(NH<sub>3</sub>)<sub>4</sub>]SO<sub>4</sub>.H<sub>2</sub>O (ii) Sodium cobaltinitrite , Na<sub>3</sub>[Co(NO<sub>2</sub>)<sub>6</sub>]
  - (iii) Potassium chromioxalate , K<sub>3</sub>[Cr(C<sub>2</sub>O<sub>4</sub>)<sub>3</sub>].

### 2 Credits

### 3 credits

### CHO-418: ORGANIC GENERAL PRACTICAL-II

- 1. Preparation of benzoin, benzil and benzillic acid from benzaldehyde.
- 2. Preparation from p-idotoluene from p-toluidene.
- 3. Preparation of ethyl acetoacetate from ethyl acetate.
- 4. Estimation of nitrogen by Kjeldahl method.
- 5. Estimation of keto group by gravimetric method.
- 6. Dibenzalacetone from benzaldehyde.
- 7. Cannizaro reaction 4-chloro benzaldehyde as substrate.
- 8. Grignard reaction synthesis of triphenyl methanol from benzoic acid.

### THIRD SEMESTER

### CHI-501: INSTRUMENTAL METHOD OF ANALYSIS

#### UNIT-I SPECTROSCOPICAL METHOD

- (a) Atomic absorption and Flame emission spectral method and their application in quantitative analysis.
- (b) Molecular absorption and emission spectroscopy in quantitative analysis.
- (c) Light scattering technique including nephlometry and Raman spectroscopy.

#### UNIT-II ELECTROANALYCTICAL METHOD

Polarography: Basic principle, instrumentation, theory of current-voltage curve, Theory of diffusion current, Ilkovic equation, polarography wave and half wave potential. Application of polagoraphy. Cyclic volotametry anodic stripping voltametry, amperometry, conductrometry and ion selective electrodes.

#### UNIT-III THERMO ANALYTICAL METHODS

Thermogravimetric analysis (TGA): Principle, instrumentation, factors affecting TGA curve, derivative thermogravimetric analysis (DTGA) and application of thermogravimetric analysis, Differential thermal Analysis (DTA), instrumentation of DTA and application of DTA, Simultaneous study of TGA, DTA with examples. Differential scanning calorimetry (DSC) and thermometric titration.

BOOKS:	1.	Instrumental Method of Analysis	: H. Willard, L. Merritt, J.
			Dean & F. Settle
	2.	Analytical Chemistry (Theory and Practical)	: U.N. Dash
	3.	Quantitative Analysis	: Vogel

#### CHI-502: INORGANIC REACTION DYNAMICS

UNIT-I:

- MECHANISM OF SUBSTITUTION REACTIONS OF OCTAHEDRAL Co(III) COMPOUNDS
- 1. The nature of substitution reactions, Kinetic Application of Crystal Field Theory.
- 2. Acid hydrolysis of octahedral Co (III) complexes with reference to effect of charge, chelation, steric crowding & effects of leaving group.
- 3. Base hydrolysis of octahedral Co(III) complexes: Conjugate base mechanism, Test of conjugate base mechanism.
- 4. Anation reaction.
- 5. Substitution reaction with out cleavage of metal-ligand bond.

### UNIT-II MECHANISM OF SUBSTITUTION REACTIONS OF Pt (II) COMPLEXES

- 1. Trans Effect and its synthetic applications, Theories of Trans Effect (Polarization &  $\pi$  bonding Theories)
- 2. Effect of the following in determining the mechanism: Rate law and reaction profile, Trans effect, Effect of leaving group, Steric effect, Effect of charge, Electrophillic catalysis, Effect of nucleophile and Effect of temperature.
- 3. Trans Effect and its synthetic applications, Theories of Trans Effect (Polarization &  $\pi$  bonding Theories).
- 4. Effect of the following in determining the mechanism: Rate law and reaction profile, Trans effect, Effect of leaving group, Steric effect, Effect of charge, Electrophillic catalysis, Effect of nucleophile and Effect of temperature.

UNIT-III ELECTRON TRANSFER REACTIONS

Introduction, electron tunneling hypothesis, Marcus-Hush theory, atom transfer reactions, one and two electron transfer, inner sphere and outer sphere reaction, electron transfer through extended bridges and the hydrated electron.

- **BOOKS:** 1. Mechanisms of Inorganic Reactions : F. Basolo and R.G. Pearson
  - 2. Inorganic Chemistry : Cotton and Wilkinson (4th Ed)

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3 credits
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CHO-503:	NATURAL PRODUCTS AND SPECTROSCOPY 3 credits		
UNIT-I	(a) Alkaloids: Morphine (Structure elucidation, Synthesis, Molecular rearrangement and Stereochemistry)		
	(b) Steroid: Cholesterol (Structure elucidation, Synthesis).		
	(c) Terpenes: Abietic acid (Structure elucidation, Synthesis).		
UNIT-II	NMR: Magnetic properties of nuclei, Theory of magnetic nuclear resonance with special reference to proton, Instrumentation, Chemical shift, Simple spin-spin interaction, Shielding effects, Diamagnetic anisotropy, NOE, <sup>13</sup> C, <sup>15</sup> N, <sup>19</sup> F, <sup>31</sup> P NMR (preliminary idea).		
UNIT-III	(a) Mass spectrometry: Introduction, Mass spectrum, Determination of molecular formulae, Parent peak, Base peak, Use of molecular fragmentation, Mass spectra of some classes of compounds (hydrocarbons, alcohols, phenols, ketones, aldehydes, acids and esters)		
	(b) Problems involving UV, IR, NMR and Mass spectroscopy.		
BOOKS:	1. Chemistry of Natural products: Sharma and Agrawal2. Organic Chemistry II: I.L. Finar3. Spectroscopic Identification of Organic Compounds: Silverstein & Basselor		
CHO-504:	PERICYCLIC REACTION, PHOTOCHEMISTRY AND REAGENTS 3 credits		
UNIT-I	Pericyclic reactions: Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann Correlation diagrams. FMO and aromatic transition state concept. Electrocyclic reactions - Con-rotatory and dis-rotatory motions, 4n, 4n+2 and allyl systems. Cycloaddition reactions - Supra- and Antara-facial additions, 4n and 4n+2 systems, 2+2 additions of ketenes, 1,3 dipolar cycloadditions and cheletropic reactions. Sigmatropic rearrangements - Supra and Antara-facial shifts of H, Sigmatropic shift of carbon moieties, 3,3- and 5,5- sigmatropic rearrangements, Claisen, Cope and aza-Cope rearrangements. Fluxional tautomerism. Ene reaction.		
UNIT-II	a. First order Photochemical processes Light absorption, Fluorescence and Phosphorescence.		
	<ul> <li>Photo reactions: Dissociation, Reduction, Isomerisation, Cycloaddition, Paterno-Buchi reaction, Norrish type I and II reactions, Di-pi-methane reaction, Photochemistry of arenes.</li> </ul>		
UNIT-III	Reagents in organic synthesis: Gilman's reagent, Lithium dimethyl cuprate, Lithium diisopropyl amide, DCC, 1,3-Dithiane, Trimethyl sillyl iodide, Tri-n-butyl tin hydride, Osmium tetroxide, Selenium dioxide, Phase transfer catalysis (Crown ether, Merrifield resin, Wilkinson's catalyst), Dichloro dicyano benzoquinone (DDQ).		
BOOKS:	1. Conversion of Orbital Symmetry : Woodward & Hoffman		
	2. Organic Reactions and Orbital Symmetry : Gilchrist and Storr		
	3. Mechanism and Theory in Organic Chemistry : Lowry & Richardson		
	4. Basic Principles of Organic Chemistry : Roberts & Casserio		
CHP-505:	STATISTICAL MECHANICS & MO CALCULATION 3 Credits		
UNIT-I	CLASSICAL AND QUANTUM STATISTICAL MECHANICS		
	Concept of probability, Starling approximations, Most probable distribution, System, Phase Space, µ-Space, Y-Space, Liouville's Theorem, Statistical Equilibrium, Brief Concepts on Ensembles, Canonical, Grand Canonical and Micro-canonical ensembles. Bose-Einstien statistics, Fermi-Dirac statistics and Maxwell-Boltzmann statistics, Comparison of the statistics and application to the radiation and electron gas in metal.		

### M. Sc. Courses of Study

#### UNIT-II PARTITION FUNCTIONS

Significance of partition function, Calculation of thermodynamic properties and equilibrium constant in terms of partition functions, Evaluation of transnational, vibrational and rotational partition function for monoatomic and polyatomic ideal gases, electronic partition function.

Some thermal characteristics of crystalline solids, Classical treatment of solids, Einstein Model, Debye Modification, Limitation and modification of Debye theory.

#### UNIT-III STATISTICAL THERMODYNAMIC PROPERTIES OF IDEAL GASES & SOLIDS

Introduction, Ideal Monoatomic Gas, Thermodynamic Function of Monoatomic Gas, Diatomic Gases, The residual Entropies.

Some thermal characteristics of crystalline solids, Classical treatment of solids, Einstein Model, Debye Modification, Limitation and modification of Debye theory, Complex solids, Electronic Heat Capacity of Solids.

#### CHP-506: SPECTROSCOPY-I

#### **3 Credits**

#### UNIT-I: ATOMIC SPECTROSCOPY

The electromagnetic spectrum, A general discussion on various molecular excitation processes, Spectra of hydrogen and hydrogen like atoms, alkali metals spectra, L-S coupling, Term symbols, Space quantisation, Zeeman effect, Stark effect, Paschen-Back effect.

#### VIBRATIONAL AND ROTATIONAL SPECTROSCOPY UNIT-II

Molecular Spectra of Diatomic Gases, Classification of molecules, Rotational Spectra, Vibrational Spectra, Vibrational-Rotational Spectra, P, Q and R Branches.

#### UNIT-III RAMAN SPECTROSCOPY

1.

Theory of Raman spectra, Rotational Raman spectra, Vibrational Raman spectra, Rotational-Vibrational Raman spectra, comparison with IR spectra.

#### BOOKS:

- Text Book of Physical Chemistry Vol-1-4 Physical Chemistry
- 2. Physical Chemistry 3.
- Physical Chemistry Through Problems 4.
- 5. Physical Chemistry Principles & Problems
- Statistical Thermodynamics
- 6.
- 7. : Walker & Straw
- 8. 9.
  - Fundamentals of Molecular Spectroscopy : C.N. Banwell
- Fundamentals of Molecular Spectroscopy 10. : G.M. Barrow

#### CHP-507: PHYSICAL GENERAL PRACTICAL-I

- 1. Determination of ionization constants of weak acids and verification of Oswald's Dilution law.
- Verification of Onsager's Limiting law. 2.
- Conductometric titration of a mixture of HCI+CH<sub>3</sub>COOH with NaOH 3.
- Determination of solubility product of BaSO<sub>4</sub>. 4
- Potentiometric titration of strong acid with strong base. 5.
- Verification of Beer's Lambert Law and unknown concentration determination. 6.
- Verification of additivity rule spectrophotometrically. 7

#### CHP-508: PHYSICAL GENERAL PRACTICAL-II

- Determination of temperature coefficient and energy of activation of hydrolysis of ethyl 1. acetate.
- 2. To determine the rate constant of base hydrolysis of ester titrometrically.
- To study the complex formation between ammonia and Cu<sup>+2</sup>. 3.
- To study of an equilibrium  $KI + I_2 = KI_3$ . 4
- To study the simultaneous equilibria in benzoic acid benzene water system. 5.
- Determination of unknown dextrose solution by polarimetry 6.
- 7. Study of inversion of cane sugar in acid medium by polarimetry.

Experimental Physical Chemistry BOOK:

: Das and Behera

2 Credits

#### 2 Credits

: K.L. Kapoor

- : D.N. Bajpai
- : A.W. Atkins
- : Dogra & Dogra
- : Jain & Jabuhar
- : M. C. Gupta
- An Introduction to Statistical Thermodynamics: T.L. Hill
- Spectroscopy Vol. I & II

### FOURTH SEMESTER (GENERAL)

### CHG-551: BIOMOLECULES

3 credits

UNIT-I: AMINO ACIDS AND PROTEINS

Classification and functions of amino acids and proteins, Chemical reactions of amino acids, alkali titration of amino acids, Synthesis of peptides, Primary, secondary, tertiary and quaternary structures of proteins.

UNIT-II: LIPIDS

Classification and Function of lipids, Structural lipids in membranes, lipids with specific biological activities, Resolution and Analysis of lipids, Biological membrane and transport.

- UNIT-III: NUCLEIC ACIDS Structure and Function of nucleotides and nucleic acids, Replication, Transcription and Translation processes, Sequencing of nucleic acids, Genetic code, Recombinant DNA.
- **BOOKS:** 1. Principles of Biochemistry : A. L. Lehninger, D. L. Nelson and M. Cox 2. Biochemistry : L. Stryer

### CHG-552: SPECTROSCOPY-II

### 3 credits

- UNIT-I: ELECTRON SPIN RESONANCE SPECTROSCOPY Theory, instrumentation, g-values, hyperfine splitting, ESR spectra of systems with more than one unpaired electrons, double resonance, ENDOR and ELDOR techniques.
- UNIT-II: PHOTOELECTRON SPECTROSCOPY Basic principle, Instrumentation: the basic design of photoelectron spectrophotometer, X-ray photoelectron spectrophotometer, ultraviolet photoelectron spectrophotometer, chemical information from photoelectron spectroscopy, ultraviolet photoelectron spectra and their interpretation, application of X-ray photoelectron spectroscopy, auger lines.
- UNIT-III: MOSSBAUER SPECTROSCOPY Principles of Mossbauer spectroscopy, Experimental methods, Theoretical aspects, Quadrupole splitting, Magnetic hyperfine interaction.

### BOOKS:

- 1. Spectroscopy Vol. I & II : Walker & Straw
- 2. Fundamentals of Molecular Spectroscopy: C.N. Banwell
- 3. Molecular Spectroscopy: P.S. Sindhu
- 4. Fundamentals of Molecular Spectroscopy: G.M. Barrow
- 5. Physical Chemistry through problems : Dogra & Dogra

#### CHC-553: COMPUTER APPLICATION IN CHEMISTRY

UNIT-I: INTRODUCTION TO COMPUTERS

Basic structure of a computer: The CPU, the I/O devices, the internal memory, commonly used secondary storage media. Data representation: Overview of binary, octal and hexadecimal number system. The software: Concept of low level and high level languages, Compiler interpreter, editor, operating system concepts, salient features of MS-DOS. Windows operating systems.

#### UNIT-II: PROGRAMME DEVELOPMENT PROCESS

Algorithm, Flowchart, Decision-table, elements of high level programming languages. Inputoutput statements, conditional statements, control structure, concept of data file, file operations like searching, storing, with reference to Fortran/C Programming.

Fortran 77/C: Types of data, variable, input and output statement, loop, Nested loop, subscript variable. PROGRAMME DEVELOPMENT PROCESS

UNIT-III:

- a. Development of small computer codes involving simple formulae in chemistry, such as-Vander Waals equation, pH titration, Kinetics, Radiation decay.
- b. Evaluation of lattice energy and ionic radii from experimental data. Linear simultaneous equations to solve secular equations within the Huckel theory.

#### BOOKS: 1. Computational Chemistry 2. Microcomputer Quantum Mechar

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- Microcomputer Quantum Mechanics : J.P. Killngbeck
- Computer Programming in Fortran-IV : V. Rajaraman
- 4. An Introduction to Digital Computer design: V. Rajaraman and
  - T. Radhakrishnan

: A.C. Norris

5. Computer Aids to Chemistry : Ed. G. Vernin & M. Chanon

### CHC-554: PRACTICAL ON COMPUTER IN CHEMISTRY

- 1. Use of computer programmes like MS Word, EXCEL, Lotus, FOXPRO.
- 2. Execution of the Software to solve problems.
- 3. Development of small programmes for solving chemical problems.

#### CHG-555: SYNTHETIC PRACTICAL

- 1. Preparation of indigo from anthranilic acid.
- 2. Preparation of cinnamic acid from benzaldehyde.
- 3. Preparation from flavone from o-hydroxy acetophenone.
- 4. Estimation of sulfur in isothiouronium chloride prepared from thiourea.
- 5. Preparation of Styrylpyridinium dye.
- 6. Separation of components from a mixture by TLC and column chromatography.
- 7. Isolation of lactose and casein from milk.
- 8. Isolation of caffein from tea leaf
- 9. Estimation of formaldehyde
- 10. Determination of reducing sugar
- 11. Estimation of amino acid.
- 12. Hippuric acid from cow-urine

#### CHG-556: Analytical Practical

- 1. Determine the pK value of an acid-base indicator.
- 2. To estimate metal ions by spectrophotometric titration.
- 3. Simultaneous estimation of Mn and Cr in a solution of  $KMnO_4$  and  $K_2Cr_2O_7$ .
- 4. To study the stability constant of a metal complex.
- 5. Determination of composition of a complex by Job's method.
- 6. Estimation of Fe ion in a solution of Mhor's salt.
- 7. To determine the pH of a given solution by spectrphotometrically.
- 8. Acid hydrolysis of ethylacetate conductometrically.
- 9. Determination of hydrolysis constant of aniline hydrochloride.
- 10. Determination of ionisation constants of multibasic acid potentiometrically.
- 11. Determination of amount of copper from EDTA

# **INORGANIC CHEMISTRY (ELECTIVE)**

2 credits

2 credits

2 credits

2 credits

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UNIT-I:

### CHI-511: ORGANOMETALLIC CHEMISTRY

3 credits

- (a) Synthesis, uses and trends in organo metallic compounds of  $\pi$ -bonding organic ligands.
  - (b) Compounds with two electron donor ligands: Olefinic and Acetylenic complexes.
  - (c) Compounds with three electron donor ligands: Allylic complexes.
  - (d) Compounds with four electron donor ligands: Butadiene complexes.
- *UNIT-II:* Compounds with five electron ligands: h<sup>5</sup> Cyclopentadienyl, acyclic pentadienyl h<sup>5</sup> complexes, h<sup>5</sup> complexes of cyclohexadienyl, heptadienyl molecules, (b) compounds with 6-electron ligands : h<sup>6</sup> complexes of Benzene and it's derivatives, n<sup>6</sup> complexes of cyclopentatriene and cyclo octatriene .

### UNIT-III: ORGANOMETALLIC COMPOUNDS AND HOMOGENEOUS CATALYTIC REACTIONS Coordinating unsaturation, acid base behaviour of metal complexes, oxidative addition reaction, stereochemistry and mechanism of addition, insertion reactions, inytamolecular hydrogen transfer, isomerization, hydrogenation of alkenes, hydroformylation, Zigler-Natta polymerization, Alkene metathesis.

**BOOKS:** Advanced Comprehensive Inorganic Chemistry : Cotton and Wilkinson **BOOKS FOR REFERENCE:** 

- 1. Principle of Organometallic Chemistry: Coutes, Green, Powell & Wade.
- 2. Organometallic Chemistry: Pauson.
- 3. Selected Topics in Modern Chemistry: Rochow.
- 4. Modern Aspects of Inorganic Chemistry: Emelius and Sharpe.
- 5. Organometallic Chemistry: R. C. Meherhotras

# CHI-512: ANALYTICAL CHEMISTRY

#### 3 credits

*RELIABILITY OF ANALYTICAL DATA* Errors in chemical analysis, classification of errors, significant figures, precision and accuracy, methods of expressing accuracy, absolute error and relative error, methods of expressing precision, average deviation, standard deviation, confidence limits, median value, range, coefficient of variation.

Sampling in analysis definition: Theory of sampling, technique of sampling, statistical criteria of good sampling and required size, stratified sampling, transition and storage samples.

UNIT-II: SOLVENT EXTRACTION AND ION EXCHANGE

 a. <u>Solvent extraction</u>: basic principles, classification of extraction, mechanism of extraction, extraction equilibria, technique of extraction, applications in analytical chemistry.

b. <u>*lon exchange:*</u> synthesis and characteristics of ion exchange, ion exchange equilibrla, technique of ion exchange, application of ion exchange for separation.

#### UNIT-III: ULTRAVIOLET AND VISIBLE SPECTROPHOTOMETRY Introduction, nature of absorbing species, visual colorimetry, photo-electric cell and filters, Photoelectric filter photometry, errors in photoelectric photometry, Spectrophotometry, working of spectrophotometer, simultaneous spectrophotometry, differential spectrophotometry, reflectance spectrophotometry, photometric titrations, composition of coloured complex Sandell's sensitivity, relative concentration and Ringbon's plot.

### BOOKS:

1. Basic Principle of Analytical Chemistry : S.M. Khopkar

# **ORGANIC CHEMISTRY (ELECTIVE)**

### CHO-521: ORGANIC SYNTHESIS-I

- UNIT-I: Synthetic design: Introduction, Retrosynthetic approach, Terminology in Retro synthetic analysis, One group disconnection, (alcohol, carbonyl compound, olefins and acids), Two group disconnections ( $\beta$ -hydroxy compounds, $\alpha$ ,  $\beta$ -unsubstituted carbonyl compounds, 1,3-dicarbonyl compounds, 1,5 dicarbonyl compounds), Synthesis of some organic molecules by disconnection approach.
- *UNIT-II:* Formation of aliphatic Carbon-nitrogen bonds: Substitution and addition of nucleophilic nitrogen, reactions of electrophilic nitrogens, rearrangement of electron deficient nitrogen.
- UNIT-III: Organometallics in synthesis: Organo lithium, organo copper compounds, organo boranes,organometallic compounds of Zinc, Cadmium and mercury organo palladium compounds.

### CHO-522: ORGANIC SYNTHESIS-II

UNIT-I: OXIDATION REDUCTION METHODS

- (a) Oxidation: Chromium (VI), Manganese (VII) oxidants, Oxidation with peracids, oxidation with hydrogen peroxide, with singlet oxygen and other oxidants.
- (b) Reduction: Catalytic hydrogenation, Reduction witih metal hydrides, the Birch reduction, the Wolff-Kischner reduction, the Cannizarro reduction, the Resenmund reduction, other reducing agent.
- **UNIT-II:** General methods of synthesis and reactions of indole, thiazole, oxazole, imidazole, pyrazole, pyrimidine and azepine.
- **UNIT-III:** Synthesis of penicillin, ATP, Cubane and α-Onocerin

### BOOKS:

- 1. Principles of Organic synthesis
- 2. Creativity in organic synthesis
- 3. Heterocyclic chemistry

: R. O. C. Norman : J. S. Bindra and R. Bindra : A R Katrizsky

### 3 credits

# PHYSICAL CHEMISTRY (ELECTIVE)

### CHP-531: PHOTOPHYSICAL CHEMISTRY

UNIT-I: INTRODUCING PHOTOCHEMISTRY & NATURE OF LIGHT AND NATURE OF MATTER

Types of electronic transitions in polyatomic molecules, Probability of transitions. The Beer–Lambert Law. Oscillator Strength, Selection rules, The Franck–Condon principle, Electronic energy states of atoms, spectroscopic terms for electronic states, orbital symmetry and molecular symmetry, and notation for excited states of organic molecules.

UNIT-II: PHYSICAL PROPERTIES OF THE ELECTRONICALLY EXCITED MOLECULES Introduction to Fluorescence: Phenomena of Fluorescence, Jablonski Diagram, Characteristics of Fluorescence Emission, Fluorescence Lifetimes and Quantum Yields, Fluorescence Anisotropy, Molecular Information from Fluorescence, Solvent and Environmental Effects: Overview of Solvent Polarity Effects, General Solvent Effects, Lippert-Mataga Equation, Specific Solvent Effects, Temperature Effects, Excited state acidity constants-pk\* values, Additional Factors that Affect Emission Spectra, Effects of Viscosity, Probe–Probe Interactions.

### UNIT-III: PHOTOPHYSICAL KINETICS OF BIMOLECULAR PROCESSES

Quenching of Fluorescence, Theory of Collisional Quenching, Derivation of the Stern-Volmer Equation, Theory of Static Quenching, Combined Dynamic and Static Quenching, Examples of Static and Dynamic Quenching, Deviations from the Stern-Volmer Equation, Quenching Sphere of Action, Derivation of the Quenching Sphere of Action, Effects of Steric Shielding and Charge on Quenching, Fractional Accessibility to Quenchers, Applications of Quenching to Proteins and Membranes, Characteristics of Resonance Energy Transfer, Theory of Energy Transfer for a Donor–Acceptor Pair, Distance Measurements Using RET.

### BOOKS:

1.	Fundamentals of Photochemistry	:	K. K. Rohatagi-Mukherjee	
2.	Molecular Fluorescence: Principles and Applications	:	Bernard Valeur	
3.	Principles of Fluorescence Spectroscopy	:	J. R. Lakowicz	

### CHP-532: POLYMER CHEMISTRY

### UNIT-I: PROPERTIES of POLYMERS

Morphology and order in crystalline polymers-configurations of polymer chains. Crystal structure of polymers. Morphology of crystalline polymers, strain induced morphology, crystallization and melting. Polymer structure and physical properties-crystalline melting point  $T_m$  – melting point of homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature, Relationship between  $T_m$  and  $T_g$ , effects of molecular weight, diluents, chemical structure, chain topology, branching and cross linking. Property requirements and polymer utilization.

#### UNIT-II: POLYMER CHARACTERISATION Materials characterization - importance and application, Principles and general methods of compositional, structural and defect characterization, techniques of X-ray diffraction, Thermal methods - DTA, TGA, and DSC. Microscopy - optical, electron (SEM), Optical spectroscopy - UV, visible, IR and Raman spectroscopy, ESCA, NMR, particle size analysis.

UNIT-III: APPLICATION OF COMMERCIAL POLYMERS Polyethylene, polypropylene, polyvinyl Chloride, polystyrene, polybutadiene, nylons, polycarbonates, polyurethane, phenolic resins and silicone polymers – Fire retarding polymers, electrically conducting polymers and biomedical polymers.

### BOOKS:

1. Polymer Science: Gowariker, Viswanathan & Sreedhar

### 3 credits

# INDUSTRIAL CHEMISTRY (ELECTIVE)

### CHIn-541: MATERIAL AND ENERGY BALANCE

3 Credits

UNIT-I: MATERIAL BALANCE

- (a) Material Balances Without Chemical Reactions: Process Flow-Sheet, Material Balances, Recycling Operations, Material Balances of Unsteady State Operations.
- (b) Material Balances Involving Chemical Reactions, Definition of Terms, Electrochemical Reactions, Recycling, Parallel and Bypassing Operations, Metallurgical Applications

### UNIT-II: ENERGY BALANCES

Energy and Thermo-Chemistry, Energy Balances, Heat Capacity, Heat Capacity of Gases at Constant Pressure, Sensible Heat Changes in Liquids, Heat Capacity of Gaseous Mixtures, Latent Heats, Enthalpy Changes During Phase Transfers Accompanied by Sensible Heat Changes, Enthalpy Changes Accompanying Chemical Reactions, Effect of Temperature on Heat of Formation, Heat of Reaction, Adiabatic Reactions, Effect of Pressure on Heat of Reaction, Thermochemistry of Mixing Process, Dissolution of Solids, Liquid-Liquid Mixtures, Heat of Solution by Partial Molal Quantities.

UNIT III: STOICHIOMETRY AND UNIT OPERATIONS

Distillation, Absorption and Stripping, Extraction and Leaching, Crystallisation, Psychrometry, Drying, Evaporation, Less Conventional Operation

**BOOK:** Stochiometry: B I Bhatt and S. M. Vora

### CHIn-542: INDUSTRIAL PROCESSES

#### 3 Credits

- *UNIT-I:* Petroleum and coal based chemicals: Composition of petroleum, cracking processes, Commercial production of ethylene, acetylene, polymerization mechanisms, Addition, condensation, step growth, chain growth, method of polymerization, Distillation of coal.
- *UNIT-II:* (a) Oil based industries: Oils and fats: Solvent extraction of oils, hydrogenation of oil, use of oil in the manufacturing of soap, paints and varnishes.
  - (b) Surface active agents: classification and manufacturing of detergents used for cleansing purpose.
  - (c) Fermentation industries. A general discussion on fermentation conditions, manufacturing of penicillin.
- *UNIT-III:* Pesticides and Pharmaceutical industries: DDT manufacture, BHC manufacture, 2,4-D manufacture, parathion manufacture, Pharmaceutical industry
- **BOOKS:** 1. Outlines of Chemical Technology. By M. Gopala Rao and Marshall Sittig, Affiliated East-West Press Pvt. Ltd.
  - 2. Industrial Chemistry. By B. K. Sharma