

DISCIPLINE CORE COURSE	
SEMESTER - V	
CHE C 9 - T INORGANIC CHEMISTRY – III	
COURSE CREDITS	3
TOTAL CONTACT HOURS	45
DURATION OF ESA	2
FORMATIVE ASSESSMENT MARKS	40
SUMMATIVE ASSESSMENT MARKS	60

#### UNIT-I

15h

Chemical Bonding- VSEPR model, shapes of molecules- $\text{ClF}_3$ ,  $\text{ICl}_4^-$ ,  $\text{TeF}_5^-$ ,  $\text{I}_3^-$ ,  $\text{TeCl}_6^{2-}$ ,  $\text{XeF}_6$ ,  $\text{SbCl}_6^{3-}$ ,  $\text{IF}_7$ ,  $\text{ReF}_7$ ,  $\text{XeF}_8^{2-}$ ,  $\text{TaF}_8^{3-}$ ; Bent rules and energetics of hybridization; electronegativity and partial ionic character; Bonds- Multicenter, Synergic and Agostic bonding. Lattice energy: Born-Landé equation, Kapustinskii equation; polarizability and partial covalent character, radius-ratio rules, structures of simple solids, Zintl-iso-electronic relationship in solids. Molecular orbital theory: LCAO and MO diagrams of heteronuclear diatomic ( $\text{CO}$ ,  $\text{NO}$ ,  $\text{HF}$ ,  $\text{ICl}$ ) and triatomic molecules ( $\text{CO}_2$  and  $\text{NO}_2^-$ ).

#### UNIT- II

15h

Chemistry of main group elements- Structure and bonding in boranes, carboranes, metallocarboranes, Wades rules, borazines, phosphazenes, S,N- compounds. Silicates- Classification, structures, isomorphous replacement, pyroxenes, layered and vitreous silicates, zeolites and molecular sieves.

HSAB concept: Basis of HSAB concept, acid-base strength, hardness and softness, symbiosis, applications of HSAB concept; Acid- base concept in non-aqueous media, reactions in  $\text{BrF}_3$ ,  $\text{N}_2\text{O}_4$ , anhydrous  $\text{H}_2\text{SO}_4$ ,  $\text{CH}_3\text{COOH}$ . Isopoly and heteropoly acids of W, Mo and V, preparations, properties, structure and applications.

Stereoisomerism- Chirality, optical activity- CD, ORD, Cotton effect, absolute configuration of metal complexes, magnetic circular dichroism.

#### UNIT-III

15h

A. M-M bond and metal atom clusters, halide clusters, bonding in  $[\text{ReCl}_8]^{2-}$ . Metal carbonyl clusters- LNCC's and HNCC's. Electron counting in carbonyl clusters, Wades-Mingos and Lauher rules.

B. Nuclear Chemistry-The atomic nucleus-elementary particles, quarks, classification of nuclides based on Z and N values, nuclear stability, nuclear potential, binding energy. Nuclear Models: Shell model-salient features, forms of the nuclear potential, filling of orbitals, nuclear configuration, Liquid drop model, Fermi gas model, Collective model and Optical model. Radioactivity, radioactive decay kinetics, Parent-daughter decay-growth relationship-secular and transient equilibria, theories of  $\alpha$ ,  $\beta^-$ ,  $\beta^+$  and  $\gamma$ -decay, internal conversion, Auger effect.

#### Recommended Books/References:

1. Basic Inorganic Chemistry- F. A. Cotton, G. Wilkinson and P. L. Gaus; John Wiley and sons. Inc, 6th edition (1999).
2. Advanced Inorganic Chemistry, 6th edition; F. A. Cotton and G. Wilkinson.
3. Inorganic Chemistry IV edition; J. E. Huheey, E. A. Keiter and R. L. Keiter, Addison; Wesley (1993).
4. Inorganic Chemistry, II edition, D. F. Shriver, P. W. Atkins and C. H. Langford, ELBS; Oxford University Press, 1994.

5. Chemistry of elements; N. N. Greenwood and A. E. Earnshaw, Butterworth Heinemann (1997).
6. Concise Inorganic Chemistry, 5th edition; J. D. Lee (1996).
7. Essentials of nuclear chemistry, 4th edition; H. J. Arniker, NAIL publishers (1995); Chapters 1, 3 and 4.
8. Nuclear and Radioactive chemistry; Friedlander, Kennedy and Miller; Chapters 8 and 9.
9. Inorganic Chemistry, 3rd Edition; Gary. L. Miessler and Donald . A. Tarr (2007).

<b>CHE C 10 - P INORGANIC CHEMISTRY PRACTICAL</b>	
COURSE CREDITS	02
CONTACT HOURS	4 HOURS/WEEK
DURATION OF ESA	03
FORMATIVE ASSESSMENT MARKS	25
SUMMATIVE ASSESSMENT MARKS	25

I - Semi micro qualitative analysis of mixtures containing two anions, two common cations and one less familiar elements: W, Mo, Ce, Th, Zr, V, U and Li.

II- Preparation and quantitative analysis of inorganic complexes:

1. Cis- and trans- potassium dioxalatodiaquachromium(III) complex [analysis of oxalate and chromium]
2. Hexamminecobalt(III)chloride [analysis of cobalt]
3. Mercury tetrathiocyanatocobaltate.
4. Preparation of pentamminechlorocobalt(III)chloride.

**Recommended Books/References:**

1. Vogel's Text book of Qualitative Chemical Analysis, J. Bassett, G. H. Jeffery and J. Mendham, ELBS (1986).
2. Vogel's text book of Quantitative Chemical Analysis, 5th Edition, J. Bassett, G. H. Jeffery and J. Mendham, and R. C. Denny, Longman Scientific and Technical (1999).
3. Inorganic Semimicro Qualitative Analysis, V. V. Ramanujam; The National Pub. Co. (1974).
4. Practical Inorganic Chemistry, G. Marr and B. W. Rockett, Von Nostrand Reinhold Co., London (1972).

DISCIPLINE CORE COURSE	
SEMESTER - V	
CHE C11 - T ORGANIC CHEMISTRY - III	
COURSE CREDITS	3
TOTAL CONTACT HOURS	45
DURATION OF ESA	2
FORMATIVE ASSESSMENT MARKS	40
SUMMATIVE ASSESSMENT MARKS	60

45hl

**UNIT-I**

Nature of Bonding in Organic Molecules; Delocalized chemical bonding: Conjugation, cross conjugation, resonance. Aromaticity. Huckel's rule of aromaticity. Aromatic systems with electron numbers other than six (including azulene, tropone, tropolone and annulenes). Antiaromaticity. Aromaticity in benzenoids, meso-ionic compounds. Homo-aromaticity. Alternant and nonalternant hydrocarbons, Energy levels in odd and even-alternant hydrocarbons, energy levels for the benzyl cation, benzyl free-radical and benzyl carbanion. Hyperconjugation. Tautomerism.

6h

**Reaction Mechanisms-I**

Generation, structure, stability and reactivity of carbocations, carbanions, carbon free radicals, carbenes and nitrenes.

Classification of reactions and mechanisms. Thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates.

Methods of determining mechanisms: Based on the structure of products, determination of the presence of intermediates, isotopic labeling, isotope effects, from stereochemical evidence.

Acids and bases: Hard and soft acids and bases. Effect of structure on the strengths of acids and bases.

6h

**Reaction Mechanisms-II**

Effect of structure on reactivity: - Resonance and field effects; steric effects. The Hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation.

Nucleophilic substitution reaction at a saturated carbon: SN1, SN2, and SET mechanisms. Effect of substrate structure, attacking nucleophile, leaving group. Ambident nucleophiles and substrates.

3h

**UNIT-II****Stereochemistry-I**

Fischer, Newman, Sawhorse and flying wedge projections and their interconversions. Optical isomerism: Elements of symmetry and chirality. D-L conventions. CIP rules, R-S and M-P conventions. Chirality in compounds with a stereogenic centre, and in allenes, alkylidene cycloalkanes and spiranes (with a stereogenic axis). Cram's and Prelog's rules.

Conformational analysis: Conformational analysis of cycloalkanes: cyclobutane, cyclopentane, cyclohexanes (monosubstituted e.g., methyl, iso-propyl, tert-butyl and di-substituted cyclohexanes e.g., dialkyl, dihalo, diols), and cycloheptane.

Nomenclature and conformations of fused rings and bridged ring systems. Prochirality: Enantiotopic and diastereotopic atoms, groups and faces.

**Carbohydrates**

Introduction. Kiliani-Fischer synthesis, Determination of configuration of the monosaccharides, conformational analysis of monosaccharides. Synthesis of amino sugars ( $\beta$ -D- Glucosamine,

8h

7h

galactosamine, N-acetylmuramic acid (NAMA), N-acetyl neuraminic acid (NANA). C- and N- glycosides. Synthesis of aldonic, uronic, aldaric acids and alditols. Structure elucidation of sucrose and maltose. Structures of lactose, gentiobiose, and meliobiose. Photosynthesis of carbohydrates.

### Unit III

8h

#### Heterocyclic compounds

Nomenclature of heterocyclic compounds. Structure, reactivity, synthesis and reactions of pyrazole, imidazole, oxazole, isoxazole, thiazole, isothiazole, pyrimidine, purine and indole. Preparation and reactions of coumarins, acridines, cinnolines and quinoxalines.

#### Vitamins

7h

Biological importance and synthesis of Vitamins A, Vitamin B1 (thiamine), Vitamin B6 (pyridoxine), folic acid, pantothenic acid, riboflavin, Vitamin C, Vitamin E (?-tocopherol), Vitamin H (biotin), Vitamins K1 and K2.

#### Recommended Books/References:

1. Advanced Organic Chemistry - Reactions, Mechanism and Structure, Jerry March, John Wiley (2008).
2. Advanced Organic Chemistry, F A Carey and R J Sundberg Plenum, (1990).
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman, (2000).
4. Structure and mechanism of Organic Chemistry, C K Ingold, Cornell University Press (1999).
5. Organic Chemistry, R T Morrison and R N Boyd, Prentice-Hall, (1998).
6. Modern Organic Reactions, H O House, Benjamin, (1972).
7. Principles of Organic Synthesis, R O C Norman and J M Coxon, Blackie Academic and Professional, (1996).
8. Stereochemistry of Organic Compounds, D Nasipuri, New-Age International, (1999).
9. Stereochemistry of Carbon Compounds, E L Eliel, S H Wilen and L N Mander, John Wiley, (1994).
10. Stereochemistry, Potapov, MIR, Moscow, 1984.
11. Organic Chemistry, Volumes I and II, I L Finar, Longman, (1999).

<b>CHE C 12 - P ORGANIC CHEMISTRY PRACTICAL</b>	
COURSE CREDITS	02
CONTACT HOURS	4 HOURS/WEEK
DURATION OF ESA	03
FORMATIVE ASSESSMENT MARKS	25
SUMMATIVE ASSESSMENT MARKS	25

### **I-Preparation (one stage)**

1. Cannizarro reaction: Benzaldehyde.
2. Fries rearrangement: Phenyl acetate.
3. Friedel-Crafts reaction: Benzene and Acetyl chloride.
4. Sandmeyer reaction: 4-Chlorotoluene from 4-toluidine.
5. Pechmann reaction: Resorcinol and ethylacetoacetate.
6. Oxidation of Cyclohexanol.
7. Preparation of S- Benzylisothiuronium chloride.
8. Synthesis of p-iodonitrobenzene
9. Synthesis of N-Phenyl-2,4-dinitroaniline.
10. Synthesis of 2,4,6-tribromoaniline.
12. Synthesis of 2,4-dichlorophenoxyacetic acid.

### **II-Qualitative analysis**

Systematic analysis and identification of organic compounds.

### **Recommended Books/References:**

1. Laboratory manual of Organic Chemistry- B. B. Dey, M V Sitaraman and T R Govindachari, Allied Publish Delhi, (1996).
2. Practical Organic Chemistry - Mann and Saunders, (1980).
3. Textbook of Practical Organic Chemistry- A. I. Vogel, (1996).
4. Textbook of Quantitative Organic Analysis- A. I. Vogel, (1996).
5. A Handbook of Organic Analysis - Clarke and Hayes, (1964).
6. Comprehensive practical organic chemistry: Preparation and quantitative Analysis, V. K. Ahluwalia, R. Aggarwal, Universities Press (India), 2000.
7. Comprehensive practical organic chemistry: Qualitative analysis, V. K. Ahluwalia, S. Dhingra, Universities Press (India), 2000.
8. An advanced course in practical chemistry, A. Ghoshal, B. Mahapatra and A. Kr. Nad, New central book Calcutta, 2000.
9. Advanced practical organic chemistry, J. Mohan, Vol. I and II, Himalaya Publishing House, 1992.
10. Practical organic chemistry (Quantitative analysis), B. B. Dey, M. V. Sitaraman and T. R. Govindachari, Publishers, New Delhi, 1992.

DISCIPLINE CORE COURSE	
SEMESTER - V	
CHE C 13 -T PHYSICAL CHEMISTRY -III	
COURSE CREDITS	3
TOTAL CONTACT HOURS	45
DURATION OF ESA	2
FORMATIVE ASSESSMENT MARKS	40
SUMMATIVE ASSESSMENT MARKS	60

45 Hours

#### UNIT-I

##### Quantum Mechanics-I

3h

Concepts of Operators: Laplacian, Hamiltonian, Linear and Hermitian operators. Angular Momentum operators and their properties. Commutation of operators. Solutions of Schrödinger wave equation for a free particle, particle in a ring, particle in a three-dimensional box. Quantum mechanical degeneracy, tunneling (no derivation). Application of Schrödinger equation to harmonic oscillator, rigid rotator. Eigenfunctions and eigenvalues of angular momentum. Ladder operator method for angular momentum.

##### Quantum Mechanics-II

12h

Schrödinger equation to hydrogen atom in spherical polar co-ordinates. Solution of  $\psi$ ,  $\theta$ ,  $\phi$  equation and statements of solution of R equation. Total wave functions of hydrogen atom. Quantum numbers and their characteristics. List of wave functions for few initial states of hydrogen like atoms. Diagrams of radial and angular wave functions. Radial and angular distribution function and their significance. Electron spin (Stern-Gerlach experiment), spin-orbital, anti-symmetry and Pauli-exclusion principle, Slater determinants. Coupling of Angular momenta. Russell-Saunders and JJ-coupling, Term symbols. Spin-orbital interaction and explanation of term multiplicities (Na-D doublet). Zeeman effect. Approximate methods: Need for approximate methods. Perturbation method. Rayleigh Schrödinger perturbation theory for time-independent non-degenerate system. Application to electron in a box under the influence of an electric field. Application to He atom. Variation theory-statement and proof. Application of variation method to particle in a one-dimensional box and He atom.

#### UNIT-II

##### Chemical Dynamics-I

15h

A. Macroscopic and microscopic kinetics, Review of theories of reaction rate-Collision theory and Transition state theory, Comparison of collision theory with transition state theory, Arrhenius equation-characteristics, Significance of energy of activation, Temperature coefficient and its evaluation. Thermodynamical formulation of reaction rates (Wyne-jones and Eyring treatment), Reaction between ions in solutions - Influence of ionic strength on reaction rates (primary and secondary salt effects).

B. Concept of Steady state kinetics, Chain reactions - chain length and chain inhibition, comparison of photochemical and thermal reactions, Mechanisms of thermal and photochemical reactions between hydrogen-bromine and hydrogen-chlorine. Comparative study of thermal and photochemical hydrogen-halogen reactions. Pyrolysis of acetaldehyde, Decomposition of ethane.

C. Kinetics of fast reactions- Introduction, Study of reactions by relaxation method (Temperature and pressure jump), flow method (Plug flow method and Stopped flow method), Flash photolysis and Shock tube method.

### UNIT-III

15h

#### Chemical Dynamics-II

D. Kinetics of homogeneous catalysis-kinetics of auto catalytic reactions, kinetics of acid-base catalysed reactions. Comparison of enzyme catalysed and chemical catalysed reactions, Mechanism (Lock and Key theory), Kinetics of enzyme catalyzed reactions - Henri-Michaelis- Menten mechanism, Significance of Michaelis-Menten constant, Lineweaver-Burk plot. Effects of enzyme concentration, pH, Temperature, Activators and Inhibitors on enzyme activity.

E. Theories of unimolecular reactions: Perrin theory, Lindemann theory, and Hinshelwood theory.

F. Surface chemistry- Types of adsorption isotherms, Effect of temperature on adsorption, Mechanical adsorption, Estimation of surface area using BET equation, Gibbs adsorption isotherm and its significance, Surface tension and surface energy, Pressure difference across curved surface (Laplace equation), Vapour pressure of droplets (Kelvin equation), Surface film on liquids (electro-kinetic phenomena), Catalytic activity of surfaces.

#### Recommended Books/References:

1. Physical Chemistry, P. W. Atkins, Julio de Paula, ELBS, 7th edition, (2002).
2. Physical Chemistry: A Molecular Approach, McQuarrie and Simon, Viva, New Delhi, (2001).
3. Introduction to Quantum Chemistry, A. K. Chandra, Tata McGraw Hill, (1988).
4. Quantum Chemistry, Ira. N. Levine, Prentice Hall, New Jersey, (1991).
5. Quantum Chemistry, R. K. Prasad, New Age International, 2nd edition, (2000).
6. Quantum Chemistry through problems and solutions, R. K. Prasad, New Age International (1997).
7. Chemical Kinetics- K. J. Laidler, McGraw Hill. Inc. New York (1988).
8. Principles of Chemical Kinetics - House J. E. Wm C Brown Publisher, Boston, (1997).
9. Kinetics and Mechanism - A. A. Frost and R. G. Pearson, John-Wiley, New York, (1961).
10. Chemical Kinetic Methods - C. Kalidas, New Age International Publisher, New Delhi (1995)
11. S.H. Maran and C. F. Pruton, 4th Edn., Oxford, & IBH publishing Co. Pvt. Ltd. New Delhi (1965).
12. Physical Chemistry- P. Atkins and J. D. Paula, 9th Edn., Oxford University Press (2010).
13. Biochemistry, - Geoffrey Zubay, 2nd Edn., Macmillan Publishing Co. New York (1981).
14. Kinetics and Mechanism of Chemical Transformations- J. Rajaraman and J. Kuriakose, Mc Millan.

<b>CHE C 14 - P PHYSICAL CHEMISTRY PRACTICAL</b>	
COURSE CREDITS	02
CONTACT HOURS	4 HOURS/WEEK
DURATION OF ESA	03
FORMATIVE ASSESSMENT MARKS	25
SUMMATIVE ASSESSMENT MARKS	25

1. Verification of Beer's Law for  $\text{Cu}^{2+}$  ions
2. Verification of Beer's Law for  $\text{Fe}^{2+}$  ions
3. Estimation of  $\text{Fe}^{2+}$  ions concentration in the given solution by titration of FAS versus  $\text{KMnO}_4$  through colorimetric method.
4. Estimation of  $\text{Fe}^{2+}$  ions concentration using EDTA through colorimetric method
5. Phase diagram of two component systems and determination of  $E_c$ ,  $E_T$  and the determination of composition of given unknown.
6. Determination of partial molar volume of solute - $\text{H}_2\text{O}$  system by apparent molar volume method.

7. Determination of the viscosity of a mixture by apparent molar volume method.

### **Conductometric Experiments**

1. Precipitation titration: conductometric titration of lithium sulphate versus BaCl<sub>2</sub>
2. Conductometric titration of weak acid versus weak base.

### **Potentiometric Experiments**

3. Determination of single electrode potential of Cu<sup>2+</sup>/Cu and estimate the given unknown concentration.
4. Determination of single electrode potential of Zn<sup>2+</sup>/Zn and estimate the given unknown concentration.
5. Titration of AgNO<sub>3</sub> versus KCl.
6. Titration of weak acid against a strong base using quinhydrone electrode and calculation of pK<sub>a</sub> and K<sub>a</sub> of the weak acid.
7. Determination of pH of a buffer by using quinhydrone electrode and comparison of the pH values obtained with glass electrode.

### **Recommended Books/References:**

1. Findlays practical physical chemistry revised by P. B. Levitt, Longman's London (1966).
2. Experiments in Physical Chemistry by Shoemaker and Garland, McGraw Hill International Edn. (1966)
3. Advanced Practical Physical Chemistry by J. B. Yadav, Goel Publications Meerut (1988)
4. Senior Practical Physical Chemistry by B. C. Kosla, Simla Printers New Delhi (1987)
5. Experimental Physical Chemistry by Daniel et al., McGraw Hill, New York (1962).
6. Practical Physical Chemistry by A.M James and P. E. Pritchard, Longman's Group Ltd (1968)
7. Experimental Physical Chemistry by Wilson, Newcombe & others, Pergamon Press, New York (1962)
8. Experimental Physical Chemistry by R. C. Behra and B Behra, Tata McGraw, New Delhi (1983)
9. Experimental Physical Chemistry by V. D. Atavale and Parul Mathur, New Age International, New York (2006)
10. Physical Chemistry Laboratory Principles and Experiments by H. W. Salberg J. I. Morrow, S. R. Cohen and Green Macmillan publishing Co .new York.
11. Practical's in physical chemistry A. Modern Approach by P.S Sindhu, Mac. Millan Publishers Delhi (2006) (1986).
15. Physical Chemistry of Surfaces- A. W. Adamson, Interscience Publisher Inc., New York (1967).
16. Surface Chemistry: Theory and Applications, J. J. Bikerman, Academic Press. New York (1972).



<b>CHE C 15-T SPECTROSCOPY - I</b>	
COURSE CREDITS	4
TOTAL CONTACT HOURS	60
DURATION OF ESA	3
FORMATIVE ASSESSMENT MARKS	40
SUMMATIVE ASSESSMENT MARKS	60

**60 Hours**

### UNIT-I

#### **Molecular spectroscopy-I**

**15h**

Interaction of electromagnetic radiation with molecules and various types of spectra; Born-Oppenheimer approximation.

Rotation spectroscopy: Selection rules, intensities of spectral lines, determination of bond lengths of diatomic and linear triatomic molecules, isotopic substitution.

Vibrational spectroscopy: Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies. Fundamental frequencies, overtones, hot bands, degrees of freedom for polyatomic molecules, modes of vibration, concept of group frequencies. Vibration-rotation spectroscopy: diatomic vibrating rotator, P, Q, R branches.

### UNIT-II

#### **Molecular spectroscopy-II**

**15h**

Raman spectroscopy: Qualitative treatment of Rotational Raman effect; Effect of nuclear spin, Vibrational Raman spectra, Stokes and anti-Stokes lines; their intensity difference, rule of mutual exclusion.

Nuclear Magnetic Resonance (NMR) spectroscopy: Principles of NMR spectroscopy, Larmor precession, chemical shift and low resolution spectra, different scales, spin-spin coupling and high resolution spectra, interpretation of PMR spectra of organic molecules. Anisotropic effects in alkene, alkyne, aldehydes and aromatics, Interpretation of NMR spectra of simple compounds. Applications of IR, UV and NMR for identification of simple organic molecules. Electron Spin Resonance (ESR) spectroscopy: Its principle, hyperfine structure, ESR of simple radicals.

### UNIT-III

#### **Organic Spectroscopy**

**15h**

General principles Introduction to absorption and emission spectroscopy.

UV Spectroscopy: Types of electronic transitions,  $\lambda_{max}$ , Chromophores and Auxochromes, Bathochromic and Hypsochromic shifts, Intensity of absorption; Application of Woodward Rules for calculation of  $\lambda_{max}$  for the following systems:  $\alpha, \beta$  unsaturated aldehydes, ketones, carboxylic acids and esters; Conjugated dienes: alicyclic, homoannular and heteroannular; Extended conjugated systems (aldehydes, ketones and dienes); distinction between cis and trans isomers.

IR Spectroscopy: Fundamental and non-fundamental molecular vibrations; IR absorption positions of O, N and S containing functional groups; Effect of H-bonding, conjugation, resonance, and ring size on IR absorptions; Fingerprint region and its significance; application in functional group analysis.

## UNIT-IV

<b>Elemental analysis:</b> Mass spectrometry (electrical discharges).	<b>6h</b>
<b>Atomic spectroscopy:</b> Atomic absorption, Atomic emission, and Atomic fluorescence. Excitation and getting sample into gas phase (flames, electrical discharges, plasmas), Wavelength separation and resolution (dependence on technique), Detection of radiation (simultaneous/scanning, signal noise), Interpretation (errors due to molecular and ionic species, matrix effects, other interferences).	
<b>X-ray analysis and electron spectroscopy (surface analysis)</b>	<b>3h</b>
<b>Radiochemical Methods</b>	<b>3h</b>
<b>Electroanalytical Methods:</b> Potentiometry & Voltammetry	<b>3h</b>

### Recommended Books/References:

1. Laideler K. J. and Meiser J. M. Physical Chemistry Third Edition (International)1999
2. Levine I. N., Physical Chemistry, Fourth Edition), McGraw-Hill (International), 1995.
3. McQuarrie D. A. and Simon J. D. Physical Chemistry- A Molecular Approach, University Science Books, 1998.
4. P.W. Atkins: Physical Chemistry.
5. G.W. Castellan: Physical Chemistry.
6. Banwell, C. N. & McCash, E. M. Fundamentals of Molecular Spectroscopy 4th Ed.Tata McGraw-Hill: New Delhi (2006).
7. Brian Smith: Infrared Spectral Interpretations: A Systematic Approach.
8. Kemp, W. Organic Spectroscopy, Palgrave
9. Principles of Instrumental Analysis - 6th Edition by Douglas A. Skoog, F. James Holler, and Stanley Crouch (ISBN 0-495-01201-7).
10. Instrumental Methods of Analysis, 7th ed, Willard, Merritt, Dean, Settle.

VOCATIONAL	
CHE V1-T: MOLECULAR MODELLING & DRUG DESIGN	
COURSE CREDITS	3
TOTAL CONTACT HOURS	45
DURATION OF ESA	2
FORMATIVE ASSESSMENT MARKS	40
SUMMATIVE ASSESSMENT MARKS	60

45 Hours

### UNIT – I

#### Introduction to Molecular Modelling

7h

Introduction. Useful Concepts in Molecular Modelling: Coordinate Systems. Potential Energy Surfaces. Molecular Graphics. Surfaces. Computer Hardware and Software. The Molecular Modelling Literature.

Force Fields: Fields. Bond Stretching. Angle Bending. Introduction to nonbonded interactions. Electrostatic interactions. van der Waals Interactions. Hydrogen bonding in Molecular Mechanics. Force Field Models for the Simulation of Liquid Water.

8h

### UNIT – II

#### Energy Minimization and Computer Simulation

7h

Minimization and related methods for exploring the energy surface. Non-derivative method, First and second order minimization methods. Computer simulation methods. Simple thermodynamic properties and Phase Space. Boundaries. Analyzing the results of a simulation and estimating Errors.

#### Molecular Dynamics & Monte Carlo Simulation

8h

Molecular Dynamics Simulation Methods. Molecular Dynamics using simple models. Molecular Dynamics with continuous potential. Molecular Dynamics at constant temperature and pressure. Metropolis method. Monte Carlo simulation of molecules. Models used in Monte Carlo simulations of polymers.

### UNIT - III

#### Structure Prediction and Drug Design

15h

Structure prediction - Introduction to comparative Modeling. Sequence alignment. Constructing and evaluating a comparative model. Predicting protein structures by 'Threading', Molecular docking. Structure based de novo ligand design, Drug Discovery – Chemoinformatics – QSAR.

#### Recommended Books/References:

1. Leach, A.R. Molecular Modelling Principles and Application, Longman, 2001.
2. Haile, J.M. Molecular Dynamics Simulation Elementary Methods, John Wiley and Sons, 1997.
3. Gupta, S.P. QSAR and Molecular Modeling, Springer - Anamaya Publishers, 2008.

<b>PRACTICAL- CHE V1 LAB: MOLECULAR MODELLING &amp; DRUG DESIGN</b>	
COURSE CREDITS	02
CONTACT HOURS	4 HOURS/WEEK
DURATION OF ESA	03
FORMATIVE ASSESSMENT MARKS	25
SUMMATIVE ASSESSMENT MARKS	25

- 1) Compare the optimized C-C bond lengths in ethane, ethene, ethyne and benzene. Visualize the molecular orbitals of the ethane  $\sigma$  bonds and ethene, ethyne, benzene and pyridine  $\pi$  bonds.
- 2) (a) Perform a conformational analysis of butane. (b) Determine the enthalpy of isomerization of cis and trans 2-butene.

**OR**

- 3) Visualize the electron density and electrostatic potential maps for LiH, HF, N<sub>2</sub>, NO and CO and comment. Relate to the dipole moments. Animate the vibrations of these molecules.
- 4) (a) Relate the charge on the hydrogen atom in hydrogen halides with their acid character. (b) Compare the basicities of the nitrogen atoms in ammonia, methylamine, dimethylamine and trimethylamine.

**OR**

- 5) (a) Compare the shapes of the molecules: 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol. Note the dipole moment of each molecule. (b) Show how the shapes affect the trend in boiling points: (118 °C,, 100 °C,, 108 °C, 82 °C, respectively).
- 6) Build and minimize organic compounds of your choice containing the following functional groups. Note the dipole moment of each compound: (a) alkyl halide (b) aldehyde (c) ketone (d) amine (e) ether (f) nitrile (g) thiol (h) carboxylic acid (i) ester (j) amide.

**OR**

- 7) (a) Determine the heat of hydration of ethylene. (b) Compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.
- 8) Arrange 1-hexene, 2-methyl-2-pentene, (E)-3-methyl-2-pentene, (Z)-3-methyl-2-pentene, and 2,3-dimethyl-2-butene in order of increasing stability.

**OR**

- 9) (a) Compare the optimized bond angles H<sub>2</sub>O, H<sub>2</sub>S, H<sub>2</sub>Se. (b) Compare the HAH bond angles for the second row dihydrides and compare with the results from qualitative MO theory.
- 10) Note: Software: ChemSketch, ArgusLab ([www.planaria-software.com](http://www.planaria-software.com)), TINKER 6.2 ([dasher.wustl.edu/ffe](http://dasher.wustl.edu/ffe)), WebLab Viewer, Hyperchem, or any similar software.

#### **Recommended Books/References:**

1. Leach, A.R. Molecular Modelling Principles and Application, Longman, 2001.
2. Haile, J.M. Molecular Dynamics Simulation Elementary Methods, John Wiley and Sons, 1997.
3. Gupta, S.P. QSAR and Molecular Modeling, Springer - Anamaya Publishers, 2008.

<b>VOCATIONAL</b>	
<b>CHE V1-T: GREEN CHEMISTRY</b>	
COURSE CREDITS	3
TOTAL CONTACT HOURS	45
DURATION OF ESA	2
FORMATIVE ASSESSMENT MARKS	40
SUMMATIVE ASSESSMENT MARKS	60

**45 Hours**

### UNIT-I

#### **Introduction to Green Chemistry**

**3h**

What is Green Chemistry? Need for Green Chemistry. Goals of Green Chemistry. Limitations/ Obstacles in the pursuit of the goals of Green Chemistry

Principles of Green Chemistry and Designing a Chemical synthesis

**12h**

Twelve principles of Green Chemistry with their explanations and examples and special emphasis on the following:

Designing a Green Synthesis using these principles; Prevention of Waste/ byproducts; maximum incorporation of the materials used in the process into the final products , Atom Economy, calculation of atom economy of the rearrangement, addition, substitution and elimination reactions.

- Prevention/ minimization of hazardous/ toxic products reducing toxicity. risk = (function) hazard × exposure; waste or pollution prevention hierarchy.
- Green solvents– supercritical fluids, water as a solvent for organic reactions, ionic liquids, fluoruous biphasic solvent, PEG, solventless processes, immobilized solvents and how to compare greenness of solvents.
- Energy requirements for reactions – alternative sources of energy: use of microwaves and ultrasonic energy.
- Selection of starting materials; avoidance of unnecessary derivatization – careful use of blocking/protecting groups.
- Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; catalysis and green chemistry, comparison of heterogeneous and homogeneous catalysis, biocatalysis, asymmetric catalysis and photocatalysis.
- Prevention of chemical accidents designing greener processes, inherent safer design, principle of ISD “What you don’t have cannot harm you”, greener alternative to Bhopal Gas Tragedy (safer route to carcarbaryl) and Flixiborough accident (safer route to cyclohexanol) subdivision of ISD, minimization, simplification, substitution, moderation and limitation.
- Strengthening/ development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

### UNIT-II

#### **Examples of Green Synthesis/ Reactions and some real world cases - I**

**15h**

1. Green Synthesis of the following compounds: adipic acid, catechol, disodium iminodiacetate (alternative to Strecker synthesis)

2. Microwave assisted reactions in water: Hofmann Elimination, methyl benzoate to benzoic acid, oxidation of toluene and alcohols; microwave assisted reactions in organic solvents Diels-Alder reaction and Decarboxylation reaction.
3. Ultrasound assisted reactions: sonochemical Simmons-Smith Reaction (Ultrasonic alternative to Iodine)
4. Surfactants for carbon dioxide – replacing smog producing and ozone depleting solvents with CO<sub>2</sub> for precision cleaning and dry cleaning of garments.
5. Designing of Environmentally safe marine antifoulant.
6. Rightfit pigment: synthetic azopigments to replace toxic organic and inorganic pigments.

### UNIT-III

Examples of Green Synthesis/ Reactions and some real world cases - I

5h

7 . An efficient, green synthesis of a compostable and widely applicable plastic (poly lactic acid) made from corn.

8 Healthier fats and oil by Green Chemistry: Enzymatic interesterification for production of no Trans-Fats and Oils.

9 Development of Fully Recyclable Carpet: Cradle to Cradle Carpeting

10h

#### Future Trends in Green Chemistry

Oxidation reagents and catalysts; Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; co crystal controlled solid state synthesis (C2S3); Green chemistry in sustainable development.

#### Recommended Books/References:

1. Ahluwalia, V.K. & Kidwai, M.R. New Trends in Green Chemistry, Anamalaya Publishers (2005).
2. Anastas, P.T. & Warner, J.K.: Green Chemistry - Theory and Practical, Oxford University Press (1998).
3. Matlack, A.S. Introduction to Green Chemistry, Marcel Dekker (2001).
4. Cann, M.C. & Connely, M.E. Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).
5. Ryan, M.A. & Tinneland, M. Introduction to Green Chemistry, American Chemical Society, Washington (2002).
6. Lancaster, M. Green Chemistry: An Introductory Text RSC Publishing, 2nd Edition, 2010

PRACTICAL - CHE V1 LAB: GREEN CHEMISTRY	
COURSE CREDITS	02
CONTACT HOURS	4 HOURS/WEEK
DURATION OF ESA	03
FORMATIVE ASSESSMENT MARKS	25
SUMMATIVE ASSESSMENT MARKS	25

1. Safer starting materials

- Preparation and characterization of nanoparticles of gold using tea leaves.

2. Using renewable resources

- Preparation of biodiesel from vegetable/ waste cooking oil.

**OR**

3. Avoiding waste

- Preparation of propene by two methods can be studied
  - Triethylamine ion + OH<sup>-</sup> → propene + trimethylpropene + water
  - 1-Propanal H<sub>2</sub>SO<sub>4</sub>/H<sup>+</sup> → Propene + water
- Other types of reactions, like addition, elimination, substitution and rearrangement should also be studied for the calculation of atom economy.

4. Use of enzymes as catalysts

- Benzoin condensation using Thiamine Hydrochloride as a catalyst instead of cyanide.

**OR**

5. Alternative Green solvents

- Extraction of D-limonene from orange peel using liquid CO<sub>2</sub> prepared from dry ice.
- Mechanochemical solvent free synthesis of azomethines.

6. Alternative sources of energy

- Solvent free, microwave assisted one pot synthesis of phthalocyanine complex of copper (II).
- Photoreduction of benzophenone to benzopinacol in the presence of sunlight.

**Recommended Books/References:**

1. Anastas, P.T & Warner, J.C. Green Chemistry: Theory and Practice, Oxford University Press (1998).
2. Kirchoff, M. & Ryan, M.A. Greener approaches to undergraduate chemistry experiment. American Chemical Society, Washington DC (2002).
3. Ryan, M.A. Introduction to Green Chemistry, Tinnensand; (Ed), American Chemical Society, Washington DC (2002).
4. Sharma, R.K.; Sidhwani, I.T. & Chaudhari, M.K. I.K. Green Chemistry Experiment: A monograph International Publishing House Pvt Ltd. New Delhi. Bangalore CISBN 978-93-81141-55-7 (2013).
5. Cann, M.C. & Connelly, M. E. Real world cases in Green Chemistry, American Chemical Society (2008).
6. Cann, M. C. & Thomas, P. Real world cases in Green Chemistry, American Chemical Society (2008).
7. Lancaster, M. Green Chemistry: An Introductory Text RSC Publishing, 2nd Edition, 2010.
8. Pavia, D.L., Lampman, G.M., Kriz, G.S. & Engel, R.G. Introduction to Organic Laboratory Techniques: A Microscale and Macro Scale Approach, W.B.Saunders, 1995.

VOCATIONAL	
CHE V1 - T: POLYMER CHEMISTRY	
COURSE CREDITS	3
TOTAL CONTACT HOURS	45
DURATION OF ESA	2
FORMATIVE ASSESSMENT MARKS	40
SUMMATIVE ASSESSMENT MARKS	60

45 Hours

### UNIT-I

#### Introduction and history of polymeric materials

Different schemes of classification of polymers, Polymer nomenclature, Molecular forces and chemical bonding in polymers, Texture of Polymers.

3h

#### Functionality and its importance

Criteria for synthetic polymer formation, classification of polymerization processes, Relationships between functionality, extent of reaction and degree of polymerization. Bi- functional systems, Poly-functional systems.

4h

#### Kinetics of Polymerization

Mechanism and kinetics of step growth, radical chain growth, ionic chain (both cationic and anionic) and coordination polymerizations, Mechanism and kinetics of copolymerization, polymerization techniques.

4h

#### Crystallization and crystallinity

Determination of crystalline melting point and degree of crystallinity, Morphology of crystalline polymers, Factors affecting crystalline melting point.

4h

### UNIT-II

Nature and structure of polymers-Structure Property relationships. Determination of molecular weight of polymers ( $M_n$ ,  $M_w$ , etc) by end group analysis, viscometry, light scattering and osmotic pressure methods. Molecular weight distribution and its significance. Polydispersity index. Glass transition temperature ( $T_g$ ) and determination of  $T_g$ , Free volume theory, WLF equation, Factors affecting glass transition temperature ( $T_g$ ).

15h

### UNIT-III

#### Properties of Polymers (Physical, Thermal, Flow & Mechanical Properties)

Brief introduction to preparation, structure, properties and application of the following polymers: polyolefins, polystyrene and styrene copolymers, poly(vinyl chloride) and related polymers, poly(vinyl acetate) and related polymers, acrylic polymers, fluoro polymers, polyamides and related polymers. Phenol formaldehyde resins (Bakelite, Novalac), polyurethanes, silicone polymers, polydienes, Polycarbonates, Conducting Polymers, [polyacetylene, polyaniline, poly(p-phenylene sulphide polypyrrole, polythiophene)].

15h



**Recommended Books/References:**

1. Seymour, R.B. & Carraher, C.E. Polymer Chemistry: An Introduction, Marcel Dekker, Inc. New York, 1981.
2. Odian, G. Principles of Polymerization, 4th Ed. Wiley, 2004.
3. Billmeyer, F.W. Textbook of Polymer Science, 2nd Ed. Wiley Interscience, 1971.
4. Ghosh, P. Polymer Science & Technology, Tata McGraw-Hill Education, 1991.
5. Lenz, R.W. Organic Chemistry of Synthetic High Polymers. Inter science Publishers, New York, 1967.

<b>PRACTICAL - CHE V1 LAB: POLYMER CHEMISTRY</b>	
COURSE CREDITS	02
CONTACT HOURS	4 HOURS/WEEK
DURATION OF ESA	03
FORMATIVE ASSESSMENT MARKS	25
SUMMATIVE ASSESSMENT MARKS	25

**I. Polymer characterization**

1. Determination of molecular weight by viscometry:
  - (a) Polyacrylamide-aq.NaNO<sub>2</sub> solution
  - (b) (Poly vinyl propylidene (PVP) in water
2. Determination of the viscosity-average molecular weight of poly(vinyl alcohol) (PVOH) and the fraction of "head-to-head" monomer linkages in the polymer.
3. Determination of molecular weight by end group analysis: Polyethylene glycol (PEG) (OH group).
4. Testing of mechanical properties of polymers.
5. Determination of hydroxyl number of a polymer using colorimetric method.

**OR**

**II. Polymer analysis**

1. Estimation of the amount of HCHO in the given solution by sodium sulphite method.
2. Instrumental Techniques.
3. IR studies of polymers.
4. DSC analysis of polymers.
5. Preparation of polyacrylamide and its electrophoresis.

\*At least 3 experiments to be carried out.

**Recommended Books/References:**

1. F.W. Billmeyer, Textbook of Polymer Science, 3rd ed. Wiley-Interscience (1984).
2. J.R. Fried, Polymer Science and Technology, 2nd ed. Prentice-Hall (2003).
3. P. Munk & T.M. Aminabhavi, Introduction to Macromolecular Science, 2nd ed. John Wiley & Sons (2002)
4. L. H. Sperling, Introduction to Physical Polymer Science, 4th ed. John Wiley & Sons (2005)

5. M.P. Stevens, *Polymer Chemistry: An Introduction* 3rd ed. Oxford University Press (2005).
6. Seymour/ Carraher's *Polymer Chemistry*, 9th ed. by Charles E. Carraher, Jr. (2013).

<b>SEMESTER - VI</b>	
<b>CHE C 16 - T INORGANIC CHEMISTRY - IV</b>	
COURSE CREDITS	3
TOTAL CONTACT HOURS	45
DURATION OF ESA	2
FORMATIVE ASSESSMENT MARKS	40
SUMMATIVE ASSESSMENT MARKS	60

**45 Hours**

### UNIT-I

#### **Metal-Ligand equilibria in solution**

**15h**

Step-wise and overall formation constant and their relationship, trends in step-wise constant, kinetic and thermodynamic stability of metal complexes, factors affecting the stability of metal complexes with reference to the nature of the metal ion and ligand, chelate effect, macrocyclic effect and their thermodynamic origin. Determination of binary formation constant by pH metry, spectrophotometry, polarography and ion exchange methods. Structure and bonding- Structure and bonding in hydride, dihydrogen, dioxygen, isocyanide, CO, NO, N<sub>2</sub> and tertiary phosphine complexes of transition metals.

### UNIT-II

#### **Metal- ligand bonding**

**15h**

Stereoisomerism- coordination numbers 3 to 8. Crystal field theory, salient features, spectrochemical series, splitting of d-orbitals in tetragonal, square planar, trigonal bipyramidal and square-pyramidal geometry, applications of CFT- colours of transition metal complexes, magnetic properties of octahedral complex, distortion of octahedral complex, CFSE and their uses, factors affecting CFSE, limitations of CFT, experimental evidence for metal-ligand covalent bonding in complexes, nephelauxetic effect, Ligand Field Theory, MO theory: tetrahedral and octahedral complexes (including p- bonding), angular overlap model. Stereochemical non-rigidity, self assembly in supramolecular chemistry.

### UNIT-III

#### **Electronic spectra of coordination compounds**

**8h**

Spectroscopic ground states, selection rules, term symbols for dn ions, Racah parameters, Orgel, Correlation and Tanabe-Sugano diagrams, spectra of 3d metal-aqua complexes of trivalent V, Cr, divalent Mn, Co and Ni, CoCl<sub>2</sub>, calculation of Dq, B and β parameters, CT spectra. Spectral properties of Lanthanide and Actinide metal complexes.

#### **Magnetic properties of coordination compounds**

**7h**

Types of magnetic behaviour, magnetic susceptibility, and its determination- Gouy, Faraday, VSM method. Diamagnetic correction, orbital contribution, spin-orbital coupling, ferro- and antiferromagnetic coupling, spin- crossover. Magnetic properties of Lanthanide and Actinide metal complexes.

#### **Recommended Books/References:**

1. Basic Inorganic Chemistry- F. A. Cotton, G. Wilkinson and P. L. Gaus; John Wiley and sons. Inc, 6th

- edition (1999).
2. Chemistry of elements- N. N. Greenwood and A. E. Earnshaw, Butterworth Heinemann (1997).
  3. Inorganic Chemistry IV edition; J. E. Huheey, E. A. Keiter and R. L. Keiter, Addison; Wesley (1993).
  4. Inorganic Chemistry, II edition, D. F. Shriver, P. W. Atkins and C. H. Langford, ELBS; Oxford University Press, 1994.
  5. Inorganic Electronic spectroscopy, A. B. P. Lever, Elsevier. (1968).
  6. Magnetochemistry, R.L. Carlin, Springer Verlag.
  7. Electronic Absorption Spectroscopy and related Techniques, D. N. Sathyanarayana, University Press (2001).
  8. Inorganic Chemistry A Unified Approach by W. W. Porterfield, Elsevier 2005 2<sup>nd</sup> edition.
  9. Textbook of inorganic chemistry by G. S. Sodhi, Viva books Pvt. Ltd (2011).

<b>CHE C 17 - P INORGANIC CHEMISTRY PRACTICAL</b>	
COURSE CREDITS	02
CONTACT HOURS	4 HOURS/WEEK
DURATION OF ESA	03
FORMATIVE ASSESSMENT MARKS	25
SUMMATIVE ASSESSMENT MARKS	25

#### **I-Gravimetric analysis**

1. Gravimetric determination of Fe in iron ore as Fe<sub>2</sub>O<sub>3</sub>.
2. Gravimetric determination of Ni in Cu and Ni solution.
3. Gravimetric determination of Fe in Fe and Cr solution.
4. Total gravimetric estimation of Fe and Al.
5. Gravimetric estimation of Cu in Cu and Fe solution.
6. Gravimetric estimation of Cu in Cu and Zn solution.

#### **II-Volumetric analysis**

7. Volumetric estimation of Ca and Mg in Dolomite solution.
8. Volumetric estimation of Cu in Cu and Ni (German Silver).
9. Volumetric estimation of Fe in Cu and Fe solution.
10. Volumetric estimation of Zn in Cu and Zn solution.
11. Volumetric estimation of Ni in Ni and Zn solution.

#### **Recommended Books/References:**

1. Vogel's text book of Quantitative Chemical Analysis, 5th Edition, J. Bassett, G. H. Jeffery and J. Mendham, and R. C. Denny, Longman Scientific and Technical (1999).
2. Practical Inorganic Chemistry, G. Marr and B. W. Rockett, Von Nostrand Reinhold Co., London (1972).

<b>SEMESTER - VI</b>	
<b>CHE C 18 - T ORGANIC CHEMISTRY – IV</b>	
COURSE CREDITS	3
TOTAL CONTACT HOURS	45
DURATION OF ESA	2
FORMATIVE ASSESSMENT MARKS	40
SUMMATIVE ASSESSMENT MARKS	60

**45 Hours**

### UNIT-I

#### **Aromatic Substitution Reactions**

**15h**

Electrophilic Substitution Reactions: 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. Effect of leaving group. Amination, sulfonylation reactions; Diazonium coupling, Vilsmeier-Haack reaction, Gatterman reaction, Gatterman-Koch reaction and Hoesch reaction.

Nucleophilic substitution reactions: The S<sub>N</sub>Ar, S<sub>N</sub>1, benzyne and S<sub>RN</sub>1 mechanisms. Reactivity: effect of substrate structure, leaving group and attacking nucleophile. Goldberg reaction, Bucherer reaction, Schiemann reaction, von Richter reaction, Sommelet-Hauser and Smiles rearrangements.

### UNIT-II

#### **Addition Reactions**

**12h**

Addition to carbon-carbon multiple bonds: mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles, and free radicals. Regio, stereo- and chemoselectivities. Orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Addition of alkenes and/or alkynes to alkenes and/or alkynes. Ene synthesis. Michael reaction.

Addition to carbon-heteroatom multiple bonds: Mechanism of metal hydride reduction (NaH, LiH, LiAlH<sub>4</sub>, NaBH<sub>4</sub>) of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents and organolithium reagents to carbonyl compounds and unsaturated carbonyl compounds. Conversion of aldehydes to nitriles. Hydrolysis of nitriles and addition of amines to isocyanates. Formation of xanthates. Wittig, Mannich and Stobbe reactions.

#### **Elimination Reactions**

**3h**

The E<sub>2</sub>, E<sub>1</sub> and E<sub>1cB</sub> mechanisms and their spectrum. E<sub>2c</sub> and E<sub>2h</sub> mechanisms. Orientation of the double bond. Reactivity-effects of substrate structure, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination reactions (including Chugaev reaction).

### UNIT-III

#### **Rearrangements**

**7h**

Wagner-Meerwein, Pinacol-Pinacolone, Fries, Wolff, Beckmann, Hofmann, Curtius, Lossen and Schmidt rearrangements. Benzil-benzilic acid rearrangement, Arndt-Eistert reaction, Tiffeneau - Demjanov reaction, Fritsch-Buttenberg-Wiechell rearrangement. Stevens, Wittig and Favorskii rearrangements,

Dienone-phenol, Baker-Venkatraman rearrangement. Baeyer-Villiger oxidation. Neber rearrangement. Benzidine rearrangement,

**Amino acids and Peptides**

Synthesis and reactions of amino acids. Classification and nomenclature of peptides. Sanger and Edman methods of sequencing. Cleavage of peptide bond by chemical and enzymatic methods. Peptide synthesis- Protection of amino group (Boc-, Z- and Fmoc-) and carboxyl group as alkyl and aryl esters. Use of DCC, EEDQ, HOBt and active esters, acid halides, anhydrides in peptide bond formation reactions. Deprotection and racemization in peptide synthesis. Solution and solid phase techniques. Synthesis of oxytocin, gramicidin, enkephalins, LH-RH. Introduction to peptidomimetics.

**Recommended Books/References:**

1. Advanced Organic Chemistry - Reactions, Mechanism and Structure, Jerry March, John Wiley (2008).
2. Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg, Plenum (1990).
3. A Guide Book to Mechanism of Organic Chemistry, Peter Sykes, Longman (2000).
4. Structure and Mechanism of Organic Chemistry, C. K. Ingold, Cornell University Press.
5. Organic Chemistry, R. T. Morrison and R. N. Boyd, Prentice-Hall (1998).
6. Modern Organic Reactions, H. O. House, Benjamin (1972).
7. Principles of Organic Synthesis, R.C. Norman and J. M. Coxon, Blackie Academic and Professional (1996).
8. Stereochemistry of Organic Compounds, D. Nasipuri, New-Age International (1999).
9. Stereochemistry of Carbon Compounds, E. L. Eliel, S. H. Wilen and L. N. Mander, John Wiley (1994).
10. Organic Chemistry, Volumes I and II, I L Finar, Longman. (1999).
11. Medicinal Chemistry, A Kar, Wiley (2000).
12. Peptides Chemistry: A practical text book, M. Bodansky, Springer-Verlag NY, 1988.
13. Solid-phase peptide synthesis: A practical approach-E. Artherton & R.C. Sheppard, I R L, Oxford Univ. Press, 1989.
14. Peptides: Chemistry and Biology, N Selwad and H.-D. Jakubke, Wiley-VCH, 2002.

CHE C 19 - P ORGANIC CHEMISTRY PRACTICAL	
COURSE CREDITS	02
CONTACT HOURS	4 HOURS/WEEK
DURATION OF ESA	03
FORMATIVE ASSESSMENT MARKS	25
SUMMATIVE ASSESSMENT MARKS	25

### Preparation (Two and three stages)

1. 2,4-Dinitrophenylhydrazine from chloronitrobenzene.
2. Anthranilic acid from phthalic acid.
3. Benzanilide from benzophenone.
4. Benzilic acid from benzoin.
5. Synthesis of Acridone.
6. Synthesis of Hydantoin.

### Quantitative analysis

7. Titrimetric estimation of amino acids.
8. Saponification value of oil.
9. Estimation of glucose by Feighling's method.
10. Estimation of keto group.
11. Estimation of phenols.
12. Iodine value of oil (chloramine-T method).

### Recommended Books/References:

1. Laboratory manual of Organic Chemistry- B. B. Dey, M V Sitaraman and T R Govindachari, Allied Publishers, New Delhi, (1996).
2. Practical Organic Chemistry - Mann and Saunders, (1980).
3. Text Book of Practical Organic Chemistry- A. I. Vogel, (1996).
4. Test Book of Quantitative Organic Analysis- A. I. Vogel, (1996).
5. Comprehensive practical organic chemistry : Preparation and quantitative Analysis, V. K. Ahluwalia, R. Aggarwal, Universities Press (India), 2000.
6. An advanced course in practical chemistry, A. Ghoshal, B. Mahapatra and A. Kr. Nad, New central book agency, Calcutta, 2000.
7. Advanced practical organic chemistry, J. Mohan, Vol. I and II, Himalaya Publishing House, 1992.
8. Practical organic chemistry (Quantitative analysis), B. B. Dey, M. V. Sitaraman and T. R. Govindachari, Allied Publishers, New Delhi, 1992.

<b>SEMESTER - VI</b>	
<b>CHE C 20 -T PHYSICAL CHEMISTRY -IV</b>	
COURSE CREDITS	3
TOTAL CONTACT HOURS	45
DURATION OF ESA	2
FORMATIVE ASSESSMENT MARKS	40
SUMMATIVE ASSESSMENT MARKS	60

**45 Hours**

### UNIT-I

#### **Thermodynamics-I**

**15h**

Thermodynamics: Concepts of partial molar properties - partial molar free energy, chemical potential, partial molar volume and its significance. Gibbs-Duhem equation, Gibbs-Duhem - Margulus equation. Determination of partial molar volume : Graphical method, intercept method and Apparent molar volume method. Concept of fugacity; Determination of fugacity by graphical method and compressibility factor method. Activity and activity coefficient : Determination of activity coefficient by EMF and solubility method. Thermodynamics of non- ideal system-Excess thermodynamic function, GE, SE, HE etc.

Phase Rule : Derivation of phase rule from the concept of chemical potential. Application of Phase Rule to three components system : Principle of triangular diagram : Plots for a mixture of three liquids consisting of one, two and three pairs of partially miscible liquids. Statistical Thermodynamics: Objectives of statistical thermodynamics, Concept of distributions, Types of ensembles. Thermodynamic probability, Most probable distribution Law

- Partition Function, (Definition and significance): Molar and molecular partitions-translational, rotational, vibrational and electronic partition functions- Relation between thermodynamic functions ( E, H, S, G and Cv ) and the partition functions.

### UNIT-II

#### **Thermodynamics-II**

**15h**

Sackur-Tetrode equation for entropy of translation function. Relation between equilibrium constant and partition function.

Different Distribution Laws: Types of Statistics : Maxwell - Boltzmann, Bose-Einstein and Fermi-Dirac statistics. Derivation of the equations for above three distribution Laws. Comparison of Bose-Einstein and Fermi-Dirac statistics with Maxwell - Boltzmann statistics. Problems and their Solutions.

Non-equilibrium Thermodynamics :

Thermodynamic criteria for non-equilibrium states-Phenomenological Laws and Onsager's reciprocity relations, Coupled and Non-coupled reactions, Entropy production and entropy flow. Electro kinetic Phenomenon.

Postulates and methodologies: Uncompensated heat and thermodynamics function production. de-Donder's inequality. Rate of entropy production. Transformations of the generalized fluxes and forces : eg., Chemical reaction, heat flow, Diffusion or material flow, flow of electric current.

### UNIT-III

#### **Electrochemistry-I**

**7h**



Electrochemistry of solutions: Ionic atmosphere, Debye-Huckel theory for the problem of activity coefficient, Debye-Huckel limiting Law, Debye-Huckel equation for appreciable concentration, Debye-Huckel Onsager conductance equation and its extension to ion solvent interactions, Debye-Huckel Bjerrum mode, Ion association, triple ions, triple ions and conductance minima. Thermodynamics of electrified interface, derivation of electro capillary Lipmann's equation, surface excess, thermodynamic aspects of surface excess. The method of determination and measurement of interfacial tension as a function of applied potential difference across the interface.

### **Electrochemistry-II**

Structure of electrified interface: Helmholtz theory, Guoy- Chapman theory, Stern model. Overpotential: Concentration overpotential and activation overpotential, Derivation of Butler- volmer equation.

Electrocatalysis: Definition and Influence of various parameters.

Quantum aspects of charge transfer at electrode solution interface, quantization of charge transfer, tunneling of electrons for hydrogen evolution with reference to electrocatalysis.

Polarography: Ilkovic equation, half wave potential and its significance, qualitative and quantitative estimation of metal ions.

Semiconductor- solution interface: Theory of double layers at semiconductor- electrolyte interface.

8h

### **Recommended Books/References:**

1. Molecular thermodynamics, Donald A. Mc Quarrie, John D. Simon University Science Books California, (1999).
2. Thermodynamics for Chemists, by S. Glasstone, East-West Press, New Delhi, (1960).
3. Thermodynamics, by Rajaraman and Kuriacose, East-West Press, (1986).
4. Statistical Thermodynamics, M. C. Gupta (Wiley Eastern Ltd.) 1993.
5. Elementary Statistical Thermodynamics, N. D. Smith, Plenum Press, NY, (1982).
6. Elements of Classical and Statistical Thermodynamics, L. K. Nash, Addison-Wiley (1979).
7. Thermodynamics, Statistical Thermodynamics and Kinetics by Thomas Engel & Philip Reid, Pearson Education inc. (2007)
8. Modern Electrochemistry Vol-1 and 2 J. O. M Bockris and A. K. N. Raddy, Plenum NewYork (1978)
9. An introduction to electrochemistry- Samuel Glasstone East-West edition New Delhi (1942)
10. Text book of physical chemistry Samuel Glasstone , 2nd edition, Mac Millan India Ltd (1991)
11. Electrochemistry, Principles and applications, Edmund, C. Potter, Cleaver-Hume press London (1961).
- 12 Principles and applications of Electrochemistry- D. R. Crow 3rd edition Chapmanhall London (1988)

CHE C 21 - P PHYSICAL CHEMISTRY PRACTICAL	
COURSE CREDITS	02
CONTACT HOURS	4 HOURS/WEEK
DURATION OF ESA	03
FORMATIVE ASSESSMENT MARKS	25
SUMMATIVE ASSESSMENT MARKS	25

1. Study the hydrolysis of methyl acetate in presence of two different concentrations of HCl and report the relative strength.
2. Study the hydrolysis of methyl acetate in the presence of HCl at different temperatures and report the energy of activation.
3. Determination of dissociation constant of a given indicator by colorimetric method.
4. Determination of degree of hydrolysis of aniline hydrochloride at room temperature and calculation of dissociation constant of the base by pH metry.
5. Study of variation of viscosity of a liquid with temperature, determine the constant A and B.
6. Analysis of a binary mixture of two miscible liquids and to determine the composition of the given unknown mixture.
7. Determination of pH of acetic acid with sodium acetate buffer by pH metry method..
8. Evaluation of Arrhenius parameter for the reaction between  $K_2S_2O_8$  versus KI (first order).

#### Conductometry

1. Acid mixture versus NaOH.
2. Weak acid with salt versus NaOH.
3. Strong acid with salt versus NaOH.
4. Determination of strength of HCl,  $CH_3COOH$  and  $CuSO_4$  versus NaOH by pH metry.
5. To determine the acidic and basic dissociation constant of an amino acid and determination of isoelectric point by pH metry.

#### Potentiometry

- 1..  $K_2Cr_2O_7$  versus FAS
2. Acid mixture versus NaOH
3. Determination of dissociation constant of  $H_3PO_4$  using potentiometric method.
4. Determination of pKa value of phosphoric acid by pH meter.

#### Recommended Books/References:

1. Findlays practical physical chemistry revised by P. B. Levitt, Longman's London (1966).
2. Experiments in Physical Chemistry by Shoemaker and Garland, McGraw Hill International Edn. (1966).
3. Advanced Practical Physical Chemistry by J. B. Yadav, Goel Publications Meerut (1988).
4. Senior Practical Physical Chemistry by B. C. Kosla, Simla Printers New Delhi (1987).
5. Experimental Physical Chemistry by Daniel et al., McGraw Hill, New York (1962).
6. Practical Physical Chemistry by A.M James and P. E. Pritchard, Longman's Group Ltd (1968)
7. Experimental Physical Chemistry by Wilson, Newcombe & others, Pergamon Press, New York (1962).
8. Experimental Physical Chemistry by R. C. Behra and B Behra, Tata McGraw, New Delhi (1983).
9. Experimental Physical Chemistry by V. D. Atavale and Parul Mathur, New Age International, New York (2001).
10. Physical Chemistry Laboratory Principles and Experiments by H. W. Salberg J. I. Morrow, S. R. Cohen and M. E.

Green Macmillan publishing Co .new York.

11. Practical's in physical chemistry A. Modern Approach by P.S Sindhu, Mac. Millan Publishers Delhi (2006).

<b>CHE 22 -T Spectroscopy - II</b>	
COURSE CREDITS	04
CONTACT HOURS	60
DURATION OF ESA	03
FORMATIVE ASSESSMENT MARKS	40
SUMMATIVE ASSESSMENT MARKS	60

**60 Hours**

#### **UNIT-I**

##### **Symmetry and Group Theory in Chemistry**

**12h**

Definition of groups, subgroups, cyclic groups, conjugate relationships, classes, simple theorems in group theory. Symmetry elements and symmetry operations, point groups, Schönflies notations, representations of groups by matrices, reducible and irreducible representations, characters of representations, Great Orthogonality Theorem (without proof) and its applications, character tables and their uses (representations for the  $C_n$ ,  $C_{nv}$ ,  $C_{nh}$ ,  $D_{nh}$  etc groups to be worked out explicitly) Mulliken symbols for irreducible representations Direct products, Applications of group theory to quantum mechanics- identifying non-zero matrix elements, derivation of the orthonormalization conditions.

Unifying principles

**3h**

Interaction of electromagnetic radiation with matter- time-dependent perturbation theory, transition moment integral, selection rules- symmetry and spin forbidden transitions

#### **UNIT-II**

##### **Infrared Spectroscopy**

**15h**

Infrared spectra of simple molecules and coordination compounds, changes in infrared spectra of donor molecules upon coordination (N,N-dimethylacetamide, urea, DMSO, pyridine N-oxide, ammine, cyano, cyanato and thiocyanato complexes), mono and multinuclear carbonyl complexes, nitrosyls, phosphine and arsine complexes. Change in spectra accompanying change in symmetry upon coordination ( $NO_3$ ,  $SO_4$ ,  $NO_2$ , and  $ClO_4$ ), hydrogen bonding. Vibration-rotation spectra of polyatomic molecules- parallel and perpendicular vibrations of linear and symmetric top molecules. Instrumentation including FTIR.

Raman spectroscopy: Theory, relation with IR spectroscopy, resonance Raman stimulated hyper and inverse Raman effects. Experimental techniques, structure determination from IR and Raman spectra.

#### **UNIT-III**

##### **Magnetic Resonance spectroscopy-I**

**15h**

Nuclear magnetic resonance spectroscopy: Magnetic properties of nuclei, population of energy levels, the Larmor precession, relaxation processes, chemical shift, shielding mechanism, spin-spin interactions, rules governing the interpretation of first order spectra, effect of chemical exchange on spectra. Analysis of complex NMR spectra, and complex metal ligands. Spin-systems: First order and second order patterns. Long range coupling : Spin decoupling, CIDNP and NOE. NMR shift reagents.

H-NMR spectra of organic molecules C-NMR (including heteronuclear coupling with F and P): Broad band and off resonance, decoupling methods, use of NMR studies of nuclei other than proton, other nuclei viz., C-NMR in structural determination of organic and inorganic molecules. F, P, B, N. Spectra of paramagnetic complexes, contact shift, double resonance technique. Instrumentation including FT-NMR. Correlation NMR spectroscopy: 1H-1H (COSY) and 13C-1H (HETEROCOSY) methods.

#### UNIT-IV

##### **Magnetic Resonance spectroscopy-II and Mo<sup>57</sup>ssbauer Spectroscopy**

7h

Electron Paramagnetic Resonance (EPR) Spectroscopy: Basic principles, selection rules, intensity, width, position of spectral line, multiplet structure of EPR spectra, hyperfine interaction, spin-orbit coupling, zero-field splitting and Kramer's degeneracy, rules for interpreting spectra, factors affecting the magnitude of values. Instrumentation. Applications to the study of free radicals, coordination compounds, biological studies and rate of electron exchange reactions.

Nuclear Quadrupole Resonance (NQR) Spectroscopy: Quadrupole nuclei, quadrupole movement, electric field gradient, the NQR experiment, structural information from NQR spectra.

##### **Mo<sup>57</sup>ssbauer Spectroscopy**

8h

Introduction, principles, conditions for Mo<sup>57</sup>ssbauer spectroscopy, parameters from Mossbauer spectra, isomer shifts, electric quadrupole interaction, magnetic exchange on spectra. Analysis of complex NMR spectra, and complex metal ligands. Spin-systems: First order and second order patterns. Long range coupling : Spin decoupling, CIDNP and NOE. NMR shift reagents. H-NMR spectra of organic molecules C-NMR (including heteronuclear coupling with F and P): Broad band and off resonance, decoupling methods, use of NMR studies of nuclei other than proton, other nuclei viz., C-NMR in structural determination of organic and inorganic molecules. F, P, B, N. Spectra of paramagnetic complexes, contact shift, double resonance technique. Instrumentation interactions, Mossbauer spectrometer. Applications in structure determination of Fe<sub>3</sub>(CO)<sub>12</sub>, Prussian blue, oxyhemerythrin, hexacyanoferrates, nitropruside, tin halides.

##### **Recommended Books/References:**

1. Chemical Applications of Group Theory, F. A. Cotton, Wiley Eastern (1976).
2. Molecular Symmetry, D. S. Schonland, Van Nostrand (1965).
3. Introduction to Molecular Spectroscopy, C. N. Banwell, TMH Edition (1994).
4. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw Hill (Int. Students Edition) (1988).
5. Molecular Spectroscopy, J. D. Graybeal, McGraw Hill (Int. Students Edition) (1990).
6. Spectroscopy, Vols. 1-3, B. P. Straughan and W. Walker, Chapman Hall (1976).
7. Physical Methods in Chemistry - R .S. Drago, Saunder college.
8. Structural Methods in Inorganic Chemistry - E. A. Ebsworth, D. W. H. Rankin and

- S.Cradock, ELBS.
9. Spectra of Inorganic and Coordination Compounds - K. Nakamoto.
  10. Infrared Spectroscopy - C.N.R. Rao.
  11. Introduction to Spectroscopy - D.L.Pavia, G.M.Lampman and G.S.Kriz, Thomson Learning, Singapore (2001)
  12. Spectroscopic Identification of organic compounds - R. M. Silverstein and F. X. Webster, 6th Edition, Wiley and Sons, India Ltd. (2006).
  13. Interpretation of Mass Spectroscopy-McLafferty.

<b>VOCATIONAL</b>	
<b>SEMESTER - VI</b>	
<b>CHE V2 - T: INORGANIC MATERIALS OF INDUSTRIAL IMPORTANCE</b>	
COURSE CREDITS	3
TOTAL CONTACT HOURS	45
DURATION OF ESA	2
FORMATIVE ASSESSMENT MARKS	40
SUMMATIVE ASSESSMENT MARKS	60

**45 Hours**

### UNIT-I

#### **Recapitulation of s- and p-Block Elements**

Periodicity in s- and p-block elements with respect to electronic configuration, atomic and ionic size, ionization enthalpy, electronegativity (Pauling, Mulliken, and Alfred-Rochow scales). Allotropy in C, S, and P. Oxidation states with reference to elements in unusual and rare oxidation states like carbides and nitrides), inert pair effect, diagonal relationship and anomalous behaviour of first member of each group.

**5h**

#### **Silicate Industries**

Glass: Glassy state and its properties, classification (silicate and non-silicate glasses). Manufacture and processing of glass. Composition and properties of the following types of glasses: Soda lime glass, lead glass, armoured glass, safety glass, borosilicate glass, fluorosilicate, coloured glass, photosensitive glass. Ceramics: Important clays and feldspar, ceramic, their types and manufacture. High technology ceramics and their applications, superconducting and semiconducting oxides, fullerenes carbon nanotubes and carbon fibre.

Cements: Classification of cement, ingredients and their role, Manufacture of cement and the setting process, quick setting cements.

**10h**

## UNIT-II

### Fertilizers

5h

Different types of fertilizers. Manufacture of the following fertilizers: Urea, ammonium nitrate, calcium ammonium nitrate, ammonium phosphates; polyphosphate, superphosphate, compound and mixed fertilizers, potassium chloride, potassium sulphate.

### Surface Coatings

10h

Objectives of coatings surfaces, preliminary treatment of surface, classification of surface coatings. Paints and pigments-formulation, composition and related properties. Oil paint, Vehicle, modified oils, Pigments, toners and lakes pigments, Fillers, Thinners, Enamels, emulsifying agents. Special paints (Heat retardant, Fire retardant, Eco-friendly paint, Plastic paint), Dyes, Wax polishing, Water and Oil paints, additives, Metallic coatings (electrolytic and electroless), metal spraying and anodizing.

## UNIT-III

### Alloys

10h

Classification of alloys, ferrous and non-ferrous alloys, Specific properties of elements in alloys. Manufacture of Steel (removal of silicon decarbonization, demanganization, desulphurization dephosphorisation) and surface treatment (argon treatment, heat treatment, nitriding, carburizing). Composition and properties of different types of steels.

### Chemical explosives

5h

Origin of explosive properties in organic compounds, preparation and explosive properties of lead azide, PETN, cyclonite (RDX). Introduction to rocket propellants.

### Recommended Books/References:

1. E. Stocchi: Industrial Chemistry, Vol-I, Ellis Horwood Ltd. UK.
2. R. M. Felder, R. W. Rousseau: Elementary Principles of Chemical Processes, Wiley Publishers, New Delhi.
3. W. D. Kingery, H. K. Bowen, D. R. Uhlmann: Introduction to Ceramics, Wiley Publishers, New Delhi.
4. J. A. Kent: Riegel's Handbook of Industrial Chemistry, CBS Publishers, New Delhi.
5. P. C. Jain & M. Jain: Engineering Chemistry, Dhanpat Rai & Sons, Delhi.
6. R. Gopalan, D. Venkappayya, S. Nagarajan: Engineering Chemistry, Vikas Publications, New Delhi.
7. B. K. Sharma: Engineering Chemistry, Goel Publishing House, Meerut

<b>CHE C 21 - P PHYSICAL CHEMISTRY PRACTICAL</b>	
COURSE CREDITS	02
CONTACT HOURS	4 HOURS/WEEK
DURATION OF ESA	03
FORMATIVE ASSESSMENT MARKS	25
SUMMATIVE ASSESSMENT MARKS	25

#### **PRACTICAL - CHE V2 LAB: INORGANIC MATERIALS OF INDUSTRIAL IMPORTANCE**

1. Determination of free acidity in ammonium sulphate fertilizer.
2. Estimation of calcium in calcium ammonium nitrate fertilizer.
3. Estimation of phosphoric acid in superphosphate fertilizer.
4. Electroless metallic coatings on ceramic and plastic material.
5. Determination of composition of dolomite (by complexometric titration).
6. Analysis of (Cu, Ni); (Cu, Zn) in alloy or synthetic samples.
7. Analysis of Cement.
8. Preparation of pigment (zinc oxide).

\* at least 3 experiments to be carried out

#### **Recommended Books/References:**

1. E. Stocchi: Industrial Chemistry, Vol-I, Ellis Horwood Ltd. UK.
2. R. M. Felder, R. W. Rousseau: Elementary Principles of Chemical Processes, Wiley Publishers, New Delhi.
3. W. D. Kingery, H. K. Bowen, D. R. Uhlmann: Introduction to Ceramics, Wiley Publishers, New Delhi.
4. J. A. Kent: Riegel's Handbook of Industrial Chemistry, CBS Publishers, New Delhi.
5. P. C. Jain, M. Jain: Engineering Chemistry, Dhanpat Rai & Sons, Delhi.
6. R. Gopalan, D. Venkappayya, S. Nagarajan: Engineering Chemistry, Vikas Publications, New Delhi.
7. Sharma, B.K. & Gaur, H. Industrial Chemistry, Goel Publishing House, Meerut (1996).

<b>VOCATIONAL</b>	
<b>CHE V2 - T: NOVEL INORGANIC SOLIDS</b>	
COURSE CREDITS	3
TOTAL CONTACT HOURS	45
DURATION OF ESA	2
FORMATIVE ASSESSMENT MARKS	40
SUMMATIVE ASSESSMENT MARKS	60

**45 Hours**

## UNIT-I

### Synthesis and modification of inorganic solids

7h

Conventional heat and beat methods, Co-precipitation method, Sol-gel methods, Hydrothermal method, Ion-exchange and Intercalation methods.

Inorganic solids of technological importance

8h

Solid electrolytes – Cationic, anionic, mixed Inorganic pigments – coloured solids, white and black pigments.

Molecular material and fullerides, molecular materials & chemistry – one-dimensional metals, molecular magnets, inorganic liquid crystals.

## UNIT-II

### Nanomaterials

7h

Overview of nanostructures and nanomaterials: classification

Preparation of gold and silver metallic nanoparticles, self-assembled nanostructures-control of nanoarchitecture-one dimensional control. Carbon nanotubes and inorganic nanowires. Bio-inorganic nanomaterials, DNA and nanomaterials, natural and antisical nanomaterials, bionano composites.

### Introduction to engineering materials for mechanical construction

8h

Composition, mechanical and fabricating characteristics and applications of various types of cast irons, plain carbon and alloy steels, copper, aluminium and their alloys like duralumin, brasses and bronzes cutting tool materials, super alloys thermoplastics, thermosets and composite materials.

## UNIT-III

### Composite materials

7h

Introduction, limitations of conventional engineering materials, role of matrix in composites, classification, matrix materials, reinforcements, metal-matrix composites, polymer-matrix composites, fibre-reinforced composites, environmental effects on composites, applications of composites.

### Specialty polymers

8h

Conducting polymers - Introduction, conduction mechanism, polyacetylene, polyparaphenylene and polypyrrole, applications of conducting polymers, Ion-exchange resins and their applications. Ceramic & Refractory: Introduction, classification, properties, raw materials, manufacturing and applications.

### Recommended Books/References:

1. Shriver & Atkins. Inorganic Chemistry, Peter Alkins, Tina Overton, Jonathan Rourke, 31 (10 Lectures)
2. Mark Weller and Fraser Armstrong, 5th Edition, Oxford University Press (2011-2012)
3. Adam, D.M. Inorganic Solids: An introduction to concepts in solid-state structural chemistry. John Wiley & Sons, 1974.
4. Poole, C.P. & Owens, F.J. Introduction to Nanotechnology John Wiley & Sons, 2003.
5. Rodger, G.E. Inorganic and Solid State Chemistry, Cengage Learning India Edition, 2002



<b>PRACTICAL - CHE V2 LAB: NOVEL INORGANIC SOLIDS</b>	
COURSE CREDITS	02
CONTACT HOURS	4 HOURS/WEEK
DURATION OF ESA	03
FORMATIVE ASSESSMENT MARKS	25
SUMMATIVE ASSESSMENT MARKS	25

1. Determination of cation exchange method
2. Determination of total difference of solids.
3. Synthesis of hydrogel by co-precipitation method.
4. Synthesis of silver and gold metal nanoparticles.

\* at least 3 experiments to be carried out

**Recommended Reference:**

1. Fahlman, B.D. Materials Chemistry, Springer, 2004.

<b>VOCATIONAL</b>	
<b>CHE V2 - T: ANALYTICAL METHODS IN CHEMISTRY</b>	
COURSE CREDITS	3
TOTAL CONTACT HOURS	45
DURATION OF ESA	2
FORMATIVE ASSESSMENT MARKS	40
SUMMATIVE ASSESSMENT MARKS	60

**45 Hours**

### UNIT-I

#### **Qualitative and quantitative aspects of analysis**

**5h**

Sampling, evaluation of analytical data, errors, accuracy and precision, methods of their expression, normal law of distribution if indeterminate errors, statistical test of data; F, Q and t test, rejection of data, and confidence intervals.

#### **Optical methods of analysis - I**

**10h**

Basic principles of quantitative analysis: estimation of metal ions from aqueous solution, geometrical isomers, keto-enol tautomers. Determination of composition of metal complexes using Job's method of continuous variation and mole ratio method.

Infrared Spectrometry: Basic principles of instrumentation (choice of source, monochromator & detector) for single and double beam instrument; sampling techniques.

Structural illustration through interpretation of data, Effect and importance of isotope substitution.

### UNIT-II

#### **Optical methods of analysis - II**

**15h**

Flame Atomic Absorption and Emission Spectrometry: Basic principles of instrumentation (choice of source, monochromator, detector, choice of flame and Burner designs. Techniques of atomization and sample introduction; Method of background correction, sources of chemical interferences and their method of removal. Techniques for the quantitative estimation of trace level of metal ions from water samples.

### UNIT-III

#### **Thermal methods of analysis**

**7h**

Theory of thermogravimetry (TG), basic principle of instrumentation. Techniques for quantitative estimation of Ca and Mg from their mixture.

#### **Electroanalytical methods**

**8h**

Classification of electroanalytical methods, basic principle of pH metric, potentiometric and conductometric titrations. Techniques used for the determination of equivalence points. Techniques used for the determination of pKa values.

Role of computers in instrumental methods of analysis.

#### **Recommended Books/References:**

1. Jeffery, G.H., Bassett, J., Mendham, J. & Denney, R.C. Vogel's Textbook of Quantitative Chemical Analysis, John Wiley & Sons, 1989.

- Willard, H.H., Merritt, L.L., Dean, J. & Settoe, F.A. Instrumental Methods of Analysis, 7th Ed. Wadsworth Publishing Company Ltd., Belmont, California, USA, 1988.
- Christian, G.D; Analytical Chemistry, 6th Ed. John Wiley & Sons, New York, 2004.
- Harris, D. C. Exploring Chemical Analysis, Ed. New York, W.H. Freeman, 2001.
- Khopkar, S.M. Basic Concepts of Analytical Chemistry. New Age, International Publisher, 2009.
- Skoog, D.A. Holler F.J. & Nieman, T.A. Principles of Instrumental Analysis,
- Cengage Learning India Ed.

<b>VOCATIONAL</b>	
<b>PRACTICAL - CHE V2 LAB: ANALYTICAL METHODS IN CHEMISTRY</b>	
COURSE CREDITS	3
TOTAL CONTACT HOURS	45
DURATION OF ESA	2
FORMATIVE ASSESSMENT MARKS	40
SUMMATIVE ASSESSMENT MARKS	60

- Determine the pH of the given aerated drinks fruit juices, shampoos and soaps.
- Determination of Na, Ca, Li in cola drinks and fruit juices using flame photometric techniques.
- Analysis of soil:
  - Determination of pH of soil.
  - Total soluble salt
  - Estimation of calcium, magnesium, phosphate, nitrate
- Spectrophotometry
  - Determination of pKa values of indicator using spectrophotometry.
  - Structural characterization of compounds by infrared spectroscopy.
  - Determination of dissolved oxygen in water.
  - Determination of chemical oxygen demand (COD).
  - Determination of Biological oxygen demand (BOD).
  - Determine the composition of the Ferric-salicylate/ ferric-thiocyanate complex by Job's method.

\* at least 3 experiments to be carried out

#### **Recommended Books/References:**

- Jeffery, G.H., Bassett, J., Mendham, J. & Denney, R.C. Vogel's Textbook of Quantitative Chemical Analysis, John Wiley & Sons, 1989.
- Willard, H.H., Merritt, L.L., Dean, J. & Settoe, F.A. Instrumental Methods of Analysis, 7th Ed. Wadsworth Publishing Company Ltd., Belmont, California, USA, 1988.
- Christian, Gary D; Analytical Chemistry, 6th Ed. John Wiley & Sons, New York, 2004.
- Harris, Daniel C: Exploring Chemical Analysis, Ed. New York, W.H. Freeman, 2001.
- Khopkar, S.M. Basic Concepts of Analytical Chemistry. New Age, International Publisher, 2009.
- Skoog, D.A. Holler F.J. & Nieman, T.A. Principles of Instrumental Analysis,
- Cengage Learning India Ed.

9. Mikes, O. Laboratory Hand Book of Chromatographic & Allied Methods, Elles
10. Harwood Series on Analytical Chemistry, John Wiley & Sons, 1979.
11. Ditts, R.V. Analytical Chemistry; Methods of Separation, van Nostrand, 1974.

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*Note: The list of experiments are suggestive. However, faculties/academic bodies may add more experiments/references or incorporate suitable revisions based on infrastructure facilities available at the Institution.*