

| Code No. | Subject Name              | Credits |
|----------|---------------------------|---------|
|          | <b>CHEMISTRY DIVISION</b> |         |
| CH101    | Applied Chemistry         | 2:0:2   |
| CH102    | Applied Chemistry Lab     | 0:0:2   |
| CH103    | Applied Chemistry         | 2:0:0   |
| CH104    | Chemistry Lab             | 0:0:2   |

### CH101 APPLIED CHEMISTRY

**Credit: 2: 0:2**  
**Marks: 50+50**

#### **Unit I : Polymers**

Homo and Heterochain polymers – types of polymerization – Addition and condensation polymerization – Effect of polymer structure on properties – Strength, plastic deformation, crystallinity, chemical resistance, plastics, thermo plastics and thermosetting plastics – moulding of plastics – biodegradable plastics.

#### **Unit II : Water Treatment**

Hardness of water, soft and hard water, units of hardness, EDTA method of estimation of hardness, softening of hard water – External Conditioning – Zeolite process, Ion exchange process – Scale and sludge formation in boilers, removal of scales – carbonate conditioning, colloidal conditioning, calgon conditioning, phosphate conditioning – desalination – water treatment for drinking purpose.

#### **Unit III : Phase Rule**

Definition and explanation of terms, advantages and limitations of phase rule, one component system – water system, two component system – reduced phase rule – thermal analysis – simple eutectic system – lead silver system, desilverisation of argentiferous lead.  
Adhesives: Advantages and disadvantages of adhesive bonding, adhesive action, physical and chemical factors influencing adhesive action – classification of adhesives.  
Lubricants: Properties of lubricants – classification – additives for lubricating oil – Greases – solid lubricants.

#### **Unit IV : Corrosion**

Chemical and electrochemical corrosion – differential aeration – factors influencing corrosion – corrosion control.

#### **Unit V : Paints**

Characteristics – constituents – their functions – mechanism of drying oil – special paints – fire retardant paints – water repellent paints – luminous paints.

#### **Metallic Coatings**

Preliminary treatment of surfaces – Hot dipping process – galvanizing, tinning – cladding – electroplating – anodizing.

#### **Text Book**

1. Daniel Yesudian C., 'Text Book of Engineering Chemistry', Hi-Tech Publications, 1999.

#### Reference Books

1. Jain P.C. & Monika Jain, 'Engineering Chemistry', Dhanpat Roy & Sons, 1991
2. Uppal M.M., 'A Text Book of Engineering Chemistry', Khanna Publications, 1988
3. Dara S.S., 'A Text Book of Engineering Chemistry', S. Chand & Co., New Delhi

### CH102 CHEMISTRY LAB

**Credit: 2: 0:2**  
**Marks: 50+50**

1. Estimation of an acid using another standard acid.
2. Estimation of a base using another standard base.
3. Estimation of Total, Permanent and Temporary hardness of water sample.
4. Estimation of Calcium and Magnesium hardness independently by EDTA.
5. Estimation of  $\text{Fe}^{2+}$  ions in rust.
6. Estimation of  $\text{Cr}^{3+}$  ions in tannery waste.
7. Determination of Percentage purity of commercial soda.
8. Determination of Percentage purity of caustic soda.
9. Estimation of available chlorine in bleaching powder.
10. Determination of Dissolved oxygen.

### CH103 APPLIED CHEMISTRY

**Credit:2:0:0**

#### Unit : I

**Polymers:-** Homo and Heterochain polymers – Types of polymerization – Addition and condensation polymerization – Effect of polymer structure on properties – strength, Plastic deformation, crystallinity, Chemical resistance, Plastics, Thermo plastics and Thermosetting plastics – Moulding of plastics – biodegradable plastics.

#### Unit : II

**Water Treatment:** Hardness of water, soft and hard water, Units of hardness, EDTA method of estimation of hardness, softening of hard water – External Conditioning – Zeolite Process, Ion exchange process – Scale and Sludge formation in boilers, Removal of Scales – Carbonate conditioning, colloidal conditioning, calgon conditioning, Phosphate conditioning – Desalination – Water treatment for drinking purpose.

#### Unit : III

**Phase rule:** Definition and explanation of terms, Advantages and limitations of phase Rule, One component system – Water system, Two component system – Reduced phase Rule – Thermal Analysis – Simple eutectic system – Lead Silver System, Desilverisation Of Argentiferrous Lead.

## Chemical Thermodynamics

*Free energy, Entropy change – law of thermodynamics – Gibbs Helmholtz equation. Third law of thermodynamics – Vant Hoff isotherm, Vant Hoff Isochore.*

### Unit : IV

**Corrosion:** Electrode potential, measurement, Nernst equation, Electrochemical series, chemical and electro chemical corrosion \_ Differential aeration \_ Factors influencing corrosion \_ corrosion control.

### Unit : V

**Paints:** Characteristics – constituents – their functions – mechanism of drying oil- Special paints – Fire retardant paints – Water repellent paints – Luminous paints.

**Metallic Coatings:** Preliminary treatment of surfaces – Hot dipping process – Galvanising, Tinning – Cladding – Electroplating – Anodising.

### Text Book:

1. Dr.C. Daniel Yesudian - 'Textbook of Engineering Chemistry', Hi-Tech Publications, 1999

### Reference Books

- 1) Jain P. C & Monika Jain - Eng. Chem., Dhanpat Roy & Sons – 1991
- 2) Uppal M.M –A Text book of Engg. Chem., Khanna Pub., 1988.
- 3) Dara S.S –A Text book of Engg. Chem., S. Chand & Co., New Delhi.
- 4) Physical chemistry – Samuel Glasstone, Macmillan II edition, 1969.
- 5) Physical Chemistry – P. L. Sony, Sulthan Chand & Sons, Delhi - 6.

## CH 104 - CHEMISTRY LAB

**Credit: 2:0:2**  
**Marks: 50 + 50**

1. Estimation of hydrochloric acid.
2. Estimation of sodium hydroxide.
3. Estimation of  $\text{Fe}^{2+}$  ions.
4. Estimation of Total, Permanent and Temporary hardness by EDTA method.
5. Estimation of Alkalinity in water sample.
6. Estimation of dissolved oxygen.
7. Estimation of sodium / calcium / potassium metal ions present in water by flame photometer.
8. Estimation of iron in water sample by spectrophotometry.
9. Conductametric estimation of an acid.
10. Potentiometric estimation of  $\text{Fe}^{2+}$  ions.

**DEPARTMENT  
OF  
SCIENCE AND HUMANITIES**

## ADDITIONAL SUBJECTS

| Code  | Subject Name         | Credits |
|-------|----------------------|---------|
| CH105 | Applied Chemistry    | 3:0:0   |
| MA212 | Discrete Mathematics | 4:0:0   |
| MA303 | Applied Mathematics  | 3:1:0   |
| PH103 | Applied Physics      | 3:0:0   |

### CH105 APPLIED CHEMISTRY

**Credit 3:0:0**

**Marks 40 + 60**

#### **UNIT I : Chemical Thermodynamics**

Thermodynamic terms – Fundamentals of thermodynamics – Heat and work – Expressions related pressure, volume and work – work done in isothermal reversible and irreversible expansion – First law of thermodynamics – Mathematical formulation of first law of thermodynamics – Second law of thermodynamics – Gibbs free energy – Entropy - Helmholtz energy and work function – Gibbs Helmholtz equation – Application – Vant Hoff Isotherm – Vant Hoff Isochore.

Material balance – Mole & Molecular weight – Avagadro's number – Stoichiometric equation – Energy balances – Enthalpy changes – Thermochemical equation and energy changes – Laws of thermo-chemistry – Heat capacity – Heat of reaction at constant volume and pressure.

#### **UNIT II : Dynamics of Chemical Process**

Rate of reaction – Determination of rate of reaction – Expression of reaction rates – Factors influencing reaction rates – Order of a reaction – Molecularity – Derivation of kinetic equations – (first order and second order) - collision theory – Activation energy and Arrhenius equation – Complex reactions – Opposing reactions, Consecutive reactions, parallel or competing reactions, Branched chain reactions leading to explosion and chain reactions) – (Explanations with example of complex reactions and no derivations) – Catalysis – Michalis – Menton equation – Derivation of Arrhenius equation.

#### **UNIT III : Electrochemistry**

Faradays law of electrolysis – Arrhenius theory of electrolytic dissociation – Conductivity of electrolyte – Measurement of electrode potential – Nernst equation for electrode potential – reference electrodes – Electrochemical cell or voltaic cell – Reversible and irreversible cells – Measurement of E.M.F of a cell – Concentration cell – Decomposition potential and polarisation.

Types of corrosion – Wet or electrochemical corrosion – Types – factors influencing corrosion – Corrosion control.

#### **UNIT IV : Water**

Sources of water – Hardness of water – Units of Hardness – Estimation of Hardness – EDTA method and Alkalinity method – Softening of hard water – Lime soda process – Zeolite process – Demineralisation or Ion exchange process – Scale and sludge formation in boilers – Internal conditioning – Boiler corrosion – Caustic embrittlement – Desalination – Water for drinking purpose.

#### **UNIT V : High Polymers**

Classification – Functionality of polymer - Mechanism (Free radical, ionic and zeigler – Nutta) – Polymerisation – Plastics – Thermoplastics and thermosetting plastics – compounding and fabrication of plastics – Important thermoplastic resins – Polythene (P.E) – Polyvinyl chloride (PVC) – Important thermosetting plastic resins – Phenolic resin Silicone resin – Industrial polymers – Nylons – Epoxy resin – Polyester resin – Applications of polymers.

#### **Text Book**

1. Dr. C. Daniel Yesudian, “Text Book of Engineering Chemistry”, Hi-Tech Publications, Mayiladuthurai, Kumbakonam – 609 001, 2003.

#### **Reference Books**

1. Jain P.C & Monika Jain, “Engineering Chemistry”, Dhanpat, 2000
2. Dara S.S, “A Text Book of Engineering Chemistry”, S. Chand & Co., New Delhi, 2002
3. P.L. Sony, “Text Book of Physical Chemistry”, Sulthan Chand & Son, Delhi, 2002

**DEPARTMENT  
OF  
CHEMISTRY**

Karunya University

## NEW SUBJECTS

| Code  | Subject Name                      | Credit |
|-------|-----------------------------------|--------|
| CH301 | Physical Chemistry – I            | 4:0:0  |
| CH302 | Analytical Chemistry – I          | 4:0:0  |
| CH303 | Organic Chemistry – I             | 4:0:0  |
| CH304 | Inorganic Chemistry – I           | 4:0:0  |
| CH305 | Inorganic Chemistry Lab (6 hours) | 0:0:4  |
| CH306 | Physical Chemistry – II           | 4:0:0  |
| CH307 | Analytical Chemistry – II         | 4:0:0  |
| CH308 | Organic Chemistry – II            | 4:0:0  |
| CH309 | Inorganic Chemistry – II          | 4:0:0  |
| CH310 | Organic Chemistry Lab (6 hours)   | 0:0:4  |
| CH311 | Physical Chemistry Lab (6 hours)  | 0:0:4  |

### CH301 PHYSICAL CHEMISTRY – I

**Credits: 4:0:0**

**Marks : 40 + 60**

#### **Unit I : Chemical thermodynamics**

The First Law of Thermodynamics - Work, heat, and energy - State functions and reversible processes - Enthalpy and applications to chemical reactions - The Second Law of Thermodynamics - Entropy and spontaneous processes - Entropy and disorder - The Third Law of Thermodynamics - entropy at absolute zero - Trouton's rule - calculation of entropy - Helmholtz and Gibbs Energies - the meaning of free energies - Maxwell relations - the standard state and calculation of thermodynamic functions - Fugacity: nonideal behavior of gases - Phase Equilibria - Chemical potential and the Gibbs phase rule - Typical phase diagrams - Clausius-Clapeyron relation - Solutions - Partial molar properties - Gibbs-Duhem equation - Ideal solution and activity of real solutions - Chemical Equilibrium - Application of thermodynamics to chemical reactions - Equilibrium constants and their calculation

#### **Unit II : Statistical thermodynamics**

Concepts of probability and Maxwell Boltzmann distribution - Basic derivation - prove that  $B = 1/KT$  - Relationship between entropy and thermodynamic probability systems with degeneracy - Definitions of partition function - applications - derivation of thermodynamic functions from partition function - entropy for monoatomic gases - Sackur - Terode equation - The Bose - Einstein's system - Basic derivation - Fermi - Dirac system - Basic derivation - negative Kelvin temperature - Heat capacity of solids - Debye and Einstein models - Thermodynamics functions of ideal gases, translational, vibrational and rotational contributions at different levels of approximation

Irreversible thermodynamics - the steady - coupled flows - application - over potential - decomposition potential - electrical double layer and electro kinetic phenomena - structure

of electrical double layer – capacity – E.K. phenomenon – steaming potential – electro dialysis – the Dom effect

### Unit III : Phase rule

Phase rule and phase equilibria – one and two components – overview – Iron, carbon equilibrium diagram – Interpretation – allotropy – heat treatment – three component system – graphical representation of systems with two salts and water.

### Unit IV : Chemical kinetics

Chemical kinetics – over view of first, second and third order reactions – rate law – complex reactions – mechanism – steady state approximation – effect of temperature – Arrhenius treatment – theories of reaction rate – collision – absolute reaction rate – competing and parallel reactions – chain reactions – transition state theory – opposing reactions – consecutive reaction – deduction of rate laws – kinetics of fast reactions – Hammetts relationship – ionic reactions in solution – effect of ionic strength.

### Unit V : Catalysis

Acid – Base catalysis – general scheme – Arrhenius complex – Vant Hoff's complex – specific and general catalysis – catalytic constants – Bronsted relationship – Hammett acidity functions – mechanism of acid-base catalysed reaction – catalysis by transition metal ions and their complexes, supported transition metal complexes as catalysts – enzyme catalysis – theory and applications

### Text books:

1. Puri, Sharma and Pathania, "Principles of Physical Chemistry", Sobhanlal Nagin chand & Co., 2002
2. K.J. Laidler, "Chemical Kinetics", Harper and Row, New York, 3<sup>rd</sup> Edition, 1990
3. Kundu and S.K. Jain, "Physical Chemistry" S. Chand & Company Ltd., New Delhi, 1984
4. P.W. Atkins, "Physical Chemistry", 5<sup>th</sup> edition, Oxford University Press, 1995

### Reference Books:

1. S. Glasstone and D.Lewis, "Elements of Physical Chemistry", 2nd Ed., 1982
2. M.J. Piling and P.W. Seakins, "Reaction Kinetics", Oxford University Press, 2<sup>nd</sup> edition, 1996
3. N.D. Smith, "Elementary Statistical Thermodynamics", Plenum Press, New York, 1982
4. J. C. Kuriacose and J.Rajaram, "Thermodynamics", Shoban Lal Nagin Chand & Co., Jalandhur, 1996
5. S Glasstone, "Thermodynamics for Chemists", Affiliated West Wes Press, New Delhi, 1965
5. B.C. McClelland, "Statistical Thermodynamics", Chapman and Hall, London, 1973
6. M. C. Gupta, "Statistical Thermodynamics", Wiley Eastern Limited, 1993
7. L.K. Nash, "Elements of classical the statistical thermodynamics", Addison-Wesley (1970)

8. C. Kalidas, "Chemical Kinetic Methods : Principles of Relaxations Techniques and application", New Age International (P) Ltd, Chennai, 1996
9. G.W. Castellan, "Physical Chemistry", Narosa Publishing house, Chennai, 1989
10. H. Snehe, "Comprehensive Physical Chemistry", Prigati Prakashan, Meerut, 1987

## CH302 ANALYTICAL CHEMISTRY – I

**Credits: 4:0:0**

**Marks : 40 + 60**

### **Unit I : Errors and the treatment of Analytical Data**

Errors, Types of errors, Minimization of determinate errors: Accuracy and Precision, Distribution of random errors, statistical treatment of finite samples – Measures of central tendency and variability, Student's confidence interval of the mean, testing for significance and criteria for rejection of an observation, control charts, propagation of errors, significant figures and computation rules, Correlation coefficient, method of least squares.

### **Unit II : Theory of volumetric and gravimetric analysis**

Acid base titrations – classification – theory of acid – based titration – neutralization – indicators – neutralization curves – choice of indicators in neutralization reactions.

Gravimetric analysis – theory of gravimetric analysis – solubility – solubility product – common ion effect – precipitation methods – co-precipitation – condition of precipitation – preparation from homogeneous solutions – purity of precipitates

General discussions of complexometric titrations, stability constants – Different ways of expressing stability of complexes, EDTA titrations – different types, masking and demasking agents, Metal ion indicators – Eriochrome Black – T, xylenol orange and murexide – Determination of hardness of water using EDTA – Determination of the following metal ions using EDTA – Zn, Mg, Ca, Mn and Ni

### **Unit III : Chromatography**

Column chromatography – Adsorption and partition – Simple elution – Stepwise or fractional elution – Gradient elution analysis – Adsorbents – Solid supports, Frontal analysis, Displacement development analysis, Ion exchange chromatography – Principle, classification and application – Elutropic series – selectivity of resins, gel chromatography, gas chromatography, gas – solid and gas – liquid – theory, technique, details of various components of apparatus – carrier gas – column – detectors – recorders – applications – molecular sieves – high performance liquid chromatography – electrophoresis & HPTLC – moisture determination – Karl Fischer titration.

### **Unit IV : Electroanalysis**

Direct potentiometry – Null point potentiometry, potentiometric titrations – Conductometric titrations - Coulometry and amperometric titrations – principle and instrumentation, primary and secondary coulometric analysis, coulometry at controlled potential – Coulometry at constant current – Separation of nickel and cobalt by coulometry

### **Unit V : Diffraction methods for structural studies**

X – ray diffraction – A brief account of the principles of molecular structure determination by X-ray diffraction from single crystal – structure factor, Phase problem and heavy atom methods, Patterson synthesis, Fourier Synthesis, Interpretation of Fourier Maps and results.

Neutron diffraction - Applications of neutron diffraction to studies of molecular structure, advantages over X- ray diffraction studies

Electron diffraction – principles of electron diffraction and applications

**Text Books:**

1. A.I. Vogel, “Textbook of quantitative analysis”, 5<sup>th</sup> edition, 1994 by G.H. Jeffery, J. Bassett, J. Mendham & R.C. Donney, ELBS, 1994
2. Douglas A. Skoog, Donald M. West and F. James Holler, “Analytical Chemistry and Introduction”, Saunders, College publishing, New York, 1990
3. Douglas A. Skoog and James J. Leary, “Principles of Instrumental Analysis”, 4<sup>th</sup> edition, Saunders, College publishing, New York, 1992
4. A.V. Ebsworth, D.W.H. Rankin and S. Cradok, “Structural Methods in Inorganic chemistry”, Blackwell Publications, ELBS, London, 1988

**Reference Books:**

1. H.A. Willard, L.L. Merrit and J.A. Dean, “Instrumental methods of Analysis”, Van Nostrand, New York, 1986
2. Gary D. Christain and James E. O’Reilly, “Instrumental analysis” 2<sup>nd</sup> edition, Prentice Hall, New Jersey, 1986
3. R.A.Day Jr., A.L. Underwood, “Quantitative Analysis”, 6<sup>th</sup> edition, Prentice Hall of India, 1993

**CH303 ORGANIC CHEMISTRY – I**

**Credits: 4:0:0**

**Marks : 40 + 60**

**Unit I : Reaction Mechanism – I**

Effect of structure and reactivity – Resonance and field effects – Steric effects – Quantitative treatments of the effect of structure and reactivity – LFER – Hammett and Taft equation – Importance of  $\sigma$  and  $\rho$  values in aromatic electrophilic substitutions – Labelling and kinetic isotopic effects.

Aromaticity – Huckel’s rule – Aromatic systems with electron numbers other than six – annulenes and hetero annulenes – Chemistry of fullerenes.

**Unit II : Reaction Mechanism – II**

Aliphatic nucleophilic substitution – mechanisms –  $S_N^2$ ,  $S_N^1$ , mixed  $S_N^1$  and  $S_N^2$ ,  $S_N^i$ , SET, neighbouring group mechanism – Reactivity – effect of substrate, attacking nucleophile, leaving group and reaction medium – Substitution at vinylic and allylic carbons.

Aromatic nucleophilic substitutions – mechanism -  $S_N^{Ar}$  -  $S_N^1$  – Benzyne – reactivity – effect of substrate, leaving group and attacking nucleophile.

### Unit III : Reaction Mechanism – III

Aromatic electrophilic substitution – Arenium ion mechanism – Orientation and reactivity in monosubstituted benzene rings – benzene rings with more than one substituent - effect of leaving group – o/p ratio.

Addition to C-C-multiple bonds – mechanisms – electrophilic, nucleophilic, free radical – orientation and reactivity – addition of conjugated systems

Elimination – mechanisms of  $\beta$  elimination – ( $E_2$ ,  $E_1$ ,  $E_{1CB}$ ) –  $E_1$  –  $E_2$  –  $E_{1CB}$  spectrum, orientation of double bonds – reactivity – effect of substrate, attacking base, leaving group and medium.

### Unit IV : Stereochemistry – I

Stereoisomerism – definitions and classification – molecular representation and inter conversion – Classification of stereo isomers – Stereoisomerism and center of chirality – molecules with a single stereogenic center – configurational nomenclature – molecules with two or more chiral centers – Stereoisomerism in cyclic compounds – axial chirality, planar chirality and helicity.

### Unit V : Stereochemistry – II

Topicity and pro stereo isomerism – Homotopic ligands and faces – enantiotopic ligands and faces – diastereotopic ligands and faces, Nomenclature of stereoheterotopic ligands and faces. Molecules with one prochiral centre – Re and Si system of nomenclature for ligands – principles of stereoselectivity – Substrate selectivity – product selectivity – asymmetric synthesis – Cram and Prelog's rule – biochemical asymmetric transformations – catalytic nexus – conformations of typical and atypical examples of substituted cyclohexanes and decalins, Klyne – Ingold - Prelog nomenclature of conformation.

#### Text Books:

1. Jerry March, "Advanced Organic Chemistry", Wiley Eastern Limited, Fourth edition, New Delhi, 1999
2. Morrison and Boyd, "Organic Chemistry", 3<sup>rd</sup> edition, United States of America, 1980
3. B. S. Bahl and Arun Bahl, "Text book of Organic Chemistry", New Delhi, S. Chand & company Ltd., 1994
4. Peterer Skyes, "A Guidebook to Mechanism in Organic Chemistry"
5. Ernest L. Eliel, "Stereochemistry of carbon compounds", 22<sup>nd</sup> reprint, Tata-McGraw Hill, New Delhi, 1997

#### Reference Books:

1. I.L. Finar, "Organic Chemistry, Volume 1: The Fundamental Principles", London Longmans, 1963
2. T.W.G. Solomons, "Organic Chemistry", Vol.2, ELBS, 1989
3. Indian Journal of Chemistry (A and B), special issues on Fullerenes, Vol. 31 A, A & B, No. 5, March 1992
4. Rai K. Bansal, "Organic reaction mechanism", Tata McGraw Hill, New Delhi, 1990
5. F.A. Cary, "Organic Chemistry", Second edition, McGraw Hill, Inc., 1992
6. P.S. Kalsi, "Stereochemistry", Wiley Eastern Limited, New Delhi, 1990

7. D. Nasipuri, "Stereochemistry of Organic Compounds – Principles and Applications" 2<sup>nd</sup> edition, New Age International, 2002
8. Accounts of Chemical Research, "Special issue on Buckminster Fullerenes", Vol. 25, No. 3, March 1992

## CH304 INORGANIC CHEMISTRY – I

Credits: 4:0:0

Marks : 40 + 60

### Unit I : Structure and Bonding

Ionic bond – Formation – Characteristics of ionic compounds, melting point, boiling point, hardness, electrical conductivity, solubility – structure of crystal lattices – Lattice energy; Born-Landé equation and Born Heber Cycle – Polarisation of ions: Fajan's rule – Calculation of some limiting ratio values – Covalent bond – Rules for covalent bond formation – Valence bond theory – Resonance and hybridization – Molecular orbital theory and its application in diatomic molecules – Comparison of VB and MO theories – The concept of multicentered bond as applied to electron deficient molecules (boron hydrides) – Bond properties – bond energy – bond length – bond polarity – electron pair repulsion theory and its applications – Hydrogen bond – types – effect on molecular properties – detection of hydrogen bonding.

### Unit II : Solids

Bond theory of solids – Electrical properties – insulators – semi conductors – superconductors – dislocation in solids – Schottky and Frenkel defects – Structure of some compounds of AX, AX<sub>2</sub> and A<sub>m</sub>X<sub>2</sub> types – perovskite, ilmenite and spinel structures

### Unit III : Nuclear Chemistry

Modes of radioactive decay and rate of radioactivity decay – Radioactive detectors – types of nuclear reactions – Artificial radioactivity – Nuclear stability – packing fraction – mass defects and binding energy – nuclear fission of uranium, liquid drop model – nuclear fusion – essential features of water coated thermal reactors and fast breeders – neutron activation analysis – carbon and rock dating – applications of tracers in chemical analysis, reaction mechanisms, medicine and industry

### Unit IV : Chemistry of Non-transition elements

Polymorphism of carbon, phosphorous and sulphur – synthesis, properties and structure of silicates, carbides, silicones, phosphazenes, sulphur – nitrogen compounds – Interhalogens and pseudohalides – oxyacids of selenium and tellurium

### Unit V : Chemistry of lanthanides and actinides

Lanthanides – position in the periodic table – general properties of lanthanides and actinides – electronic configuration, oxidation state and oxidation potential, atomic and ionic radii – Cause and consequences of lanthanide and actinide contractions – comparison of spectral and magnetic properties of lanthanide and actinide complexes – Extraction details of cerium, thorium and uranium – Chemistry of their important compounds: Oxides, nitrates and sulphates

### Text Books:

1. F.A. Cotton and G. Wilkinson, "Advanced Inorganic Chemistry", 5<sup>th</sup> edition, John Wiley and Sons, New York, 1988
2. E. Huheey James, A. Keiter Ellen and L. Keiter Richard, "Inorganic Chemistry – Principles of structure and reactivity" 4<sup>th</sup> edn., Harper Collings Publishers, New York, 1993
3. BR Puri and LR Sharma, "Principles of Inorganic Chemistry", Shoban Lal Nagin Chand and Co., 1989
4. J.D. Lee, "Concise Inorganic Chemistry", 5<sup>th</sup> edition, ELBS with Chapman and Hall, London, 1996

**Reference Books:**

1. D.E. Shriver, B.W. Atkins and C.H. Langford, "Inorganic Chemistry" 2<sup>nd</sup> edition, (ELBS), Oxford University press, 1994
2. F.A. Cotton and G. Wilkinson, "Advanced Inorganic Chemistry", 5<sup>th</sup> edition, John Wiley and Sons, New York, 1988
3. H.J. Arnikar, "Essentials of Nuclear Chemistry", 4<sup>th</sup> Ed., New Age International Publishers Ltd., New Delhi, 1995
4. B.K. Sharma, "Nuclear and Radiation Chemistry" Krishna Prakashan Media Pvt. Ltd., Meerut, 1997

**CH305 INORGANIC CHEMISTRY LAB (6 HOURS)**

**Credits: 0:0:4**

**Marks : 50 + 50**

12 experiments will be notified by the HOD from time to time

**CH306 PHYSICAL CHEMISTRY – II**

**Credits: 4:0:0**

**Marks : 40 + 60**

**Unit I : Surface Phenomena and heterogeneous catalysis**

Diffusion – adsorption – surface reaction – various adsorption isotherms - Freundlich – Langmuir – BET adsorption isotherms – derivation of BET equation – properties – modification - determination of surface area – pore volume and pore size – thermodynamics of interfaces – solid catalysts – metal – metal oxides – Geometric factor – Electronic factor zeolites – phase transfer catalysts – surface films – colloidal electrolytes – Reaction on surfaces – Mechanism of reactions ethylene, H<sub>2</sub> – Surface characterization techniques – Electron Spectroscopy for chemical analysis (ESCA) – Atomic Emission Spectroscopy (AES) – Secondary Ion Mass Spectroscopy (SIMS).

**Unit II : Mechanism of gas phase reactions**

Chemiluminescence – reactions in molecular beam – Lindemann's theory – Hinzelwood, Kassel and Slater' Treatments – abnormal frequencies – Ortho-para conversions – explosion limits – reaction rates in solution – effect of dielectric constant and ionic strength – kinetic isotope effect – linear free energy relationships – Hammett equation – Taff equation – Yukawa – Tsuno equation – fast reactions – luminescence and energy transformations – study of kinetics of stopped flow techniques – flash photolysis – shock tubes.

### **Unit III : Introduction to Materials Science**

Crystal Structure - 7 Crystal Systems - 14 Bravais Lattices - Cubic Crystals Characterization of Structure - X-ray, Electron and Neutrons diffraction - Band Theory - Semiconductors and Devices - Imperfections in Solids: Point, Line, Surface - Amorphous Solids - Inorganic Glasses (Oxides, Metallic) - Organic Glasses (Polymers)

### **Unit IV : Introduction to quantum mechanics**

The failures of classical physics – heat capacities – black body radiation – The photo electric heat – The Compton effect – The diffraction of electrons – Atomic and molecular spectra, wave particles duality – Uncertainty principle, operators and commutation relations – Postulates of quantum mechanics – Scrodinger equation, Free particle, particle in one dimensional box – Harmonic oscillator – Rigid rotor – Hydrogen atom – Angular momentum – Spin, coupling of angular momentum – Spin-orbit coupling.

### **Unit V : Quantum chemistry of atoms and molecules**

Variation and perturbation theory – Application to helium atom – Antisymmetry and Pauli's exclusion principle – Aufbau principle – Slater determinantal wave functions – Term symbols and spectroscopic states – Born Oppenheimer approximation – Hydrogen molecule ion – LCAO, MO and VB treatments of hydrogen molecule – Group theory – Character tables – Selection rules – MO treatment of large molecules with symmetry – Hybridization – Huckel theory of conjugated molecules – Cyclic systems – Woodward Hoffman rules.

#### **Text Books:**

1. Donald A McQuarrie, "Quantum Chemistry", University Science Books, Mill Valley, California, 1983.
2. AK Chandra, "Introduction to Quantum Chemistry", Tata McGraw Hill, New Delhi
3. A.W. Adamson, "Physical Chemistry of Surfaces", 5<sup>th</sup> edition, Wiley, 1990
4. C.N.R. Rao and J. Gopalakrishnan, "New Directions in Solid State Chemistry"; 2<sup>nd</sup> Edition; Cambridge University Press, 1997

#### **Reference Books:**

1. P.W. Atkins, "Molecular Quantum Mechanics", 2<sup>nd</sup> edition, Oxford University Press, 1983
2. Anthony R. West, "Solid state chemistry and it's applications", John Wiley, 1984
3. I.N. Levine, "Quantum Chemistry", 4<sup>th</sup> edition, Prentice Hall India, 1994
4. M.W. Hanna, "Quantum Mechanics in Chemistry", 3<sup>rd</sup> edition, Addison Wesley, London, 1981
5. J. Rajaram and J.C. Kuriakose, "Kinetics and mechanism of chemical transformation", McMillan India Ltd., New Delhi, 1993

## **CH307 ANALYTICAL CHEMISTRY – II**

**Credits: 4:0:0**

**Marks : 40 + 60**

### **Unit I : Atomic Spectroscopy**

Atomic absorption spectroscopy – principle – instrumentation, single and double beam atomic absorption spectrometer, detections limits and sensitivity – applications - Atomic

emission spectroscopy – Types of emission spectra – excitation energy requirement – instrumentation – spectrographs – applications - Atomic fluorescence spectroscopy.

### **Unit I I: UV – Visible Spectroscopy**

The electromagnetic spectrum – fundamental laws of photometry – deviation from Beer's law – presentation of spectra – correlation of electronic absorption spectra with molecular structure – molar absorptivity – structural effects – effect of temperature and solvents – quantitative methods – photometric titrations – electron spectroscopy for chemical analysis (ESCA)

### **Unit III : IR - spectroscopy and Raman Spectroscopy**

Selection rules for IR absorption, fundamental, overtone and hot bands – Normal modes of vibration of molecules such as carbon dioxide and water – Factors influencing the number and energy of absorption bands – Characteristic group vibrations – Factors causing shifts in group vibrations – Skeletal vibrations – Finger printing – Double beam IR spectrophotometer – Components and functions – sample handling – Nujol mull and potassium bromide pellet technique - Applications of IR spectroscopy in structural elucidation of molecules.

Raman spectroscopy – Vibrational mode – group frequencies of organic, inorganic and organometallic compounds, factors affecting the group frequencies, study of hydrogen bonding effects, vibrational spectra of ionic, coordination and metal carbonyl compounds.

### **Unit IV : Nuclear Magnetic Resonance & Electronic Spin Resonance Spectroscopy**

Basic definitions of magnetic moment and spin quantum numbers – The chemical shift – Factors affecting the magnitude of chemical shift – The TMS scale, tau and delta values – Spin – spin splitting of AB, A<sub>2</sub>B<sub>2</sub> and ABX systems – Some examples of spin – spin splitting, NMR of typical organic compounds – Ethanol, ethane, limonene, etc. – Internal rotation and NMR – Deuterium exchange reaction – NMR of nuclei other than hydrogen – mainly <sup>13</sup>C and applications – F.T. NMR and its advantages over conventional NMR

EPR – Principles, factors affecting the intensity, position and multiplet structure of the spectra – Hyperfine splitting of some simple systems, zero field splitting – Kramers degeneracy – Applications

### **Unit V : Mass Spectrometry & Thermogravimetry**

Mass spectroscopy – Basic principles – Instrumentation – The mass spectrometer – Isotope abundances – Molecular ion – Metastable ions – Fragmentation processes – Fragmentation associated with functional groups – Alkanes, alkenes, aromatic hydrocarbons, alcohols, aldehydes, carboxylic acids and esters – McLafferty rearrangement and applications – Thermogravimetry (TG) – Derivative thermogravimetry (DTG) – Differential thermal analysis (DTA) – Differential Scanning Calorimetry (DSC) – Instrumentation and applications.

Solving problems involving the techniques of Units II – V.

### **Text Books:**

1. C.N. Banwell, "Fundamentals of Molecular spectroscopy", 3<sup>rd</sup> Edn., Mc-Graw – Hill, New Delhi, 1983

- J. Dyer, "Absorption Spectroscopy of Organic Molecules", Prentice Hall of India, 3<sup>rd</sup> Edn., Macmillan, 1991
- W. Kemp, "Organic Spectroscopy", 3<sup>rd</sup> Edn., ELBS, 1991,
- Chatwal and Anand, "Instrumental methods of chemical analysis" 5th. Edition, Himalaya Publication.

**Reference Books:**

- J.K. Saunders and B.K. Hunter, "Modern NMR Spectroscopy", Oxford University Press, Oxford, 1987
- D.H. Williams and I. Fleming, "Spectroscopic methods in Organic Chemistry", 4<sup>th</sup> edition, Tata McGraw Hill, New Delhi, 1988
- R.M. Silverstein, G.C. Bassler, T.C. Morrill, "Spectrometric Identification of Organic Compounds", John Wiley, New York, 1991
- Willard, Merritt and Dean, "Instrumental Methods of Analysis", 6<sup>th</sup> Edn., Willard, H.H., 1981
- R.M. Silverstein, F.X. Webster and D.J. Kiemle, "Spectroscopic Identification of Organic Compounds", John Wiley, New York, 2003.

**CH308 ORGANIC CHEMISTRY – II**

**Credits: 4:0:0**

**Marks : 40 + 60**

**Unit I : Principles of organic synthesis**

The synthesis process – preliminary planning, molecular characteristics, functional group transformation – retrosynthetic analysis – order of events – one group – C – X disconnection – Chemo selectivity two group C-X disconnection – reversal of polarity – cyclisation reactions – protecting groups – one group disconnection C-C, alcohols, C+O, stereoselectivity – regioselectivity

**Unit II : Reagents in organic synthesis**

Use of the following reagents in organic synthesis and functional group transformations – complex metal hydrides, Gilman's reagent, lithium dimethyl cuprate, lithium diisopropyl amide (LDA), dicyclohexyl carbodimide, 1,3 – dithiane, Woodward and Prevost hydroxylation, DDO, selenium dioxide, phase transfer catalysis, crown ethers and Merrifield resin, Peterson's synthesis, Wilkinson's catalyst, Bakers yeast.

**Unit III : Pericyclic reactions**

Definition – types – FMO treatment, PMO method and correlation approaches and diagrams of typical electrocyclic reactions, cycloadditions, sigmatropic reactions – Cope and Claisen rearrangement

**Unit IV : Organic Photo Chemistry**

Introduction – Interaction of electromagnetic radiation with matter – electronic excitations – excited states – transfer of excitation energy – sensitization and quenching – photochemical eliminations, Norrish type I and II reactions, Paterno-Buchi reaction, oxidations – reductions, cis-trans isomerisation, rearrangements (di-pi methane or Zimmerman rearrangement).

### Unit V : Hetero cyclics and supramolecules

Heterocyclics – Nomenclature – compounds containing two hetero atoms – azoles – chemistry of pyrazole, imidazole, oxazole, isoxazole, thiazole and isothiazole – diazines – pyrimidines.

Supra molecular chemistry – preparation and structure of catenanes and rotaxanes – molecular recognition – synthetic applications of calixarenes and cyclodextrines – organic reactions on solid supports zeolite, clay, alumina and silica.

#### Text Books:

1. I.L. Finar, "Organic Chemistry" Vol.2, ELBS, 6<sup>th</sup> edition, Singapore, 1984
2. Robert E. Ireland, "Organic synthesis", 2<sup>nd</sup> edition, Prentice-Hall of India Pvt. Ltd., New Delhi, 1988
3. V.K. Ahluwalia and Ram Aggarwal, "Organic Synthesis", Narosa Publishing House, New Delhi
4. G.R. Chatwal, "Organic photo chemistry" 1<sup>st</sup> edition, Himalaya Publishing House, Mumbai, 1988

#### Reference Books:

1. R.O.C. Norman, "Principles of organic synthesis" 2<sup>nd</sup> edition, Chapman and Hall, London, New York, 1978
2. J.M. Coxon, B. Halton, "Organic photochemistry", Cambridge University Press, 2<sup>nd</sup> edition, 1987
3. R.K. Bansal, "Heterocyclic Chemistry", Wiley Eastern, 1990
4. Andre Loupy, "Solvent free reactions", Topics in current chemistry, Vol. 206, Page 155 –173
5. G. Schill. Catenanes, Rotaxanes, and Knots, Academic Press, New York (1971)
6. W. Carruthers, "Some modern methods of organic synthesis", Cambridge university press, 3<sup>rd</sup> edition, 1988
7. T.L. Gilchrist & R.C. Storr, "Organic reaction orbital symmetry", Cambridge university press, 1972
8. F.A. Carey and R.J. Sundberg, "Advanced Organic Chemistry Part – B: Reactions and Synthesis, Plenum Press, 3<sup>rd</sup> edition, 1990

### CH309 INORGANIC CHEMISTRY – II

Credits: 4:0:0

Marks : 40 + 60

#### Unit I : Coordination Chemistry

Introduction - Formation of complexes - Bonding theories for coordination complexes - Crystal Field Theory, Ligand Field Theory, Molecular Orbital Theory, Werner's theory – Stability constant: Experimental determination of stability constant – factors influencing – Stabilization of unusual oxidation states by complex formation – the nature of the metal – ligand bond, molecular orbital theory of a complex and its limitation – Crystal field theory – concept, influence of ligand on CF splitting and limitation – Ligand field theory – Jahn – Teller effect – electronic spectra and magnetic moments.

## Unit II : Inorganic reaction mechanisms

Reactions of square – planar complexes – Mechanism of ligand displacement reaction – Substitution in the square planar complexes - mechanism, entering group effect, cis effect and trans effect. Substitution in octahedral complexes – Dissociative and associative mechanisms – Base hydrolysis - Isomerisation reactions – Substitution without breaking the metal – ligand, electron transfer reaction – Outer sphere and inner sphere reactions.

## Unit III : Organo metallics

Definition – Types of bonds – Complexes of olefin, acetylene and cyclopentadiene and benzene derivatives – Metallocenes – Fluxional molecules – Homogeneous catalysis – Hydrogenation, carbonylation.

## Unit IV : Bio-inorganic chemistry

Essential and trace metals in biological systems – Metalloporphyrins – Chlorophyll, hemoglobin, myoglobin, vitamin B<sub>12</sub> – iron sulphur proteins – Nitrogen cycle, nitrogen fixation and dinitrogen complexes – anticancer drugs (mainly Pt complexes) and their probable mechanism of action. Metal centered enzymes – structure and function

## Unit V : Chemistry of cluster compounds and Inorganic polymers

Preparation, structure and bonding of boron hydrides, carboranes and heteroboranes – properties structure and uses of inorganic polymers of boron, silicon, germanium and tin

### Text Books:

1. BR Puri and LR Sharma, “Principles of Inorganic Chemistry”, Shoban Lal Nagin Chand and Co., 1989
2. D. Banerjee, “Coordination Chemistry”, 5<sup>th</sup> edition, ELBS with Chapman and Hall, London, 1996
3. K.K. Rohitgi Mukerjee, “Fundamentals of photochemistry’ Wiley Eastern Limited, New Delhi, 1992
4. Madan, Malik, Tuli, Inorganic Chemistry, S. Chand & Company, New Delhi

### Reference Books:

1. DR Williams, CC Thomas, RJP Williams and JRRF do Silva, “Bio-inorganic Chemistry”, New Age Publishers, India
2. Ronald D. Archer, “Inorganic and Organometallic Polymers”, Wiley-VCH, 2001
3. Florian P Pruchnik, V Pruchnik, “Organometallic Chemistry of the Transition Elements”, Springer, 1990
4. William L. Jolly, “Modern Inorganic Chemistry” 2<sup>nd</sup> Edition, McGraw-Hill, Inc. (1991)

## CH310 ORGANIC CHEMISTRY LAB (6 HOURS)

Credits: 0:0:4

Marks : 50 + 50

12 experiments will be notified by the HOD from time to time

**CH311 PHYSICAL CHEMISTRY LAB (6 HOURS)**

**Credits: 0:0:4**

**Marks : 50 + 50**

12 experiments will be notified by the HOD from time to time

Karunya University

**DEPARTMENT  
OF  
CHEMISTRY**

## ADDITIONAL SUBJECTS

| Sub. Code | Subject   | Credits |
|-----------|---|---------|
| CH106     | Applied Chemistry                               | 3:0:0   |
| CH312     | Electro-Organic Synthesis                       | 3:0:0   |
| CH313     | Advanced Electro Chemistry                      | 3:0:0   |
| CH314     | Electro Analytical Chemistry                    | 3:0:0   |
| CH315     | Materials Electro Chemistry                     | 3:0:0   |
| CH316     | Electro Deposition Techniques                   | 3:0:0   |
| CH317     | Chemistry of Energy Sources and Storage Devices | 3:0:0   |
| CH318     | Organic Chemistry                               | 3:0:0   |
| CH319     | Research Methodology in Chemistry               | 3:0:0   |

### CH106 APPLIED CHEMISTRY

**Credit: 3:0:0**

**Marks 40+60**

#### Unit I : High Polymers

**[10Hrs.]**

Classification – Functionality of polymer – Mechanism (Free radical, ionic and zeigler – Nutta) – polymerization – Plastics – Thermoplastics and Thermosetting plastics – Compounding and fabrication of plastics – Important thermoplastic resins – Polythene (P.E.) – Polyvinyl Chloride (P.V.C.) – Important thermosetting plastic resins – Phenolic resin and Silicone resin – Industrial polymers – Nylons – Epoxy resin – Polyester resin – Applications of polymers – Conducting polymers – Semi conducting Polymers

#### Unit II: Water Technology

**[8 Hrs.]**

Sources of water – Hardness of water – Units of hardness – Estimation of hardness – EDTA method and alkalinity method – Softening of hard water – Lime soda process – Zeolite process – Demineralisation or Ion exchange process – Scale and sludge formation in boilers – Internal conditioning – Boiler corrosion – Caustic embrittlement – Desalination – Water for drinking purpose

#### Unit III : Fuels and Combustion

**[12 Hrs.]**

Fuels and Classifications - gross and net calorific values - Proximate and ultimate analyses of coal – Significances – Characteristics of metallurgical coke – manufacture by Otto – Hoffman method – Synthetic petrol – Bergius process – Fischer – Tropsch's process – Knocking – Octane number – Improvement of anti knocking characteristics – Cetane number, gaseous fuels – an elementary treatment of Water gas, producer gas and CNG (definition only) – An introduction to Non-conventional Sources of Energy – Biomass – Biogas – Bio fuels (Bio-diesel and Bio-ethanol) - Theoretical calculation of calorific values (Dulong's formula) – Simple problems – Calculation of minimum air requirements – Simple problems – Flue gas analysis – Orsat's apparatus

#### Unit IV : Electrochemistry

**[10 Hrs.]**

Electrode potential – Measurement of electrode potential – Nernst equation for electrode potential – Electrochemical Series – Electrochemical cell or Voltaic cell – Concentration cell

– Primary Cell– Leclanche cell - Secondary batteries – alkaline batteries – Lead acid, and Li batteries – An introduction to Fuel Cell, H<sub>2</sub> – O<sub>2</sub> Fuel Cell – Applications  
Types of corrosion – Wet or electrochemical corrosion – Types – factors influencing corrosion – Corrosion control methods

### **Unit V : Emerging Trends in Chemistry**

**[10 Hrs.]**

Basics of Nanotechnology - Nanomaterials – Types: Nanowires, Nanotubes – Applications  
Chemical aspects of Biotechnology – Fermentation – Manufacture of ethyl alcohol and acetic acid by fermentation – Deamination  
Fundamentals of Semiconductor Technology – Semiconductor materials – Basic fabrication steps – oxidation – photolithography and etching – diffusion and ion implantation - metallization

#### **Text Book:**

1. P.C. Jain and Monika Jain, “Engineering Chemistry”, Dhanpat Rai Publishing Co. (P) Ltd., 15<sup>th</sup> Edition, 2006

#### **Reference Books:**

1. S. Glasstone and D. Lewis – “Elements of Physical Chemistry”, McMillan Co. of India Ltd., 2002
2. P.L.Soni, O.P. Dharmarsha and U.N. Dash – “Text Book of Physical Chemistry” Sulthan Chand & Sons, New Delhi, 2001
3. J C Kuriakose, and J Rajaram, “Chemistry in Engineering and Technology”, Tata Mcraw-Hill Publications Co. Ltd., New Delhi, 1996
4. V.R. Gowrikar, N.V.Viswanathan and Jaydev Sreedhar, “Polymer Science”, New Age International Pvt. Ltd., New Delhi, 2000.
5. Garry S. May and Simon M. Sze, ”Fundamentals of Semiconductor Fabrication”, Jonh Wiley & Sons, Inc., 2004, Chapter – I
6. C. Daniel Yesudian and D.G. Harris Samuel, “Materials Science & Metallurgy”, Scitech Publishers, 2004
7. Charles P. Poole Jr. and Frank J. Ownes, “Introduction to Nanotechnology”, Wiley Publishers, 2003

## **CH312 ELECTRO-ORGANIC SYNTHESIS**

**Credits: 3:0:0**

**Marks : 40 + 60**

### **Unit I:**

Principles and methods, Synthesis and mechanistic aspects of cathodic reactions of organic compounds classified by electrophores, Hydrocarbons, Nitro and related compounds, Carbonyl compounds.

### **Unit II:**

Synthetic and mechanistic aspects of anodic reactions of organic compounds classified by electrophores, Anodic oxidation of hydrocarbon, Carboxylic acids.

**Unit III:**

Electrode reactions classified by reaction type, Reductive coupling, Oxidative coupling, Cleavages and deprotection, Anodic substitution, Anodic fluorination.

**Unit IV: 4**

Stereochemistry of organic electrode processes, Amalgam and related reductions, Electrogenerated reagents, Electrogenerated acids and bases.

**Unit V:**

Present and future applications, Industrial electroorganic chemistry, Electrochemical polymerization, Chemically modified electrodes and conducting polymers.

**Text Book:**

1. M.R. Rifi, Covitz and H. Frank – Introduction to Organic Electrochemistry, ECS Princeton, 1990

**Reference Book:**

1. Sergio Trasatti, "Electrodes of Conductive Metallic Oxides". Elsevier Scientific Publishing Company, Amsterdam-Oxford-NY, 1980.

**CH313 ADVANCED ELECTROCHEMISTRY****Credits: 3:0:0****Marks : 40 + 60****UNIT I: Electrical Double Layer**

Thermodynamics of ideally polarisable and non-polarisable interfaces- Lipman equation- Determination of interfacial tension, Charge density, surface excess.

**UNIT II:**

Double layer capacitance by electro capillary & bridge methods-Helmholtz, Gouy-chapman & Stern models of the double layer Contact adsorption & its determination.

**UNIT III: Electrode Kinetics**

Concepts of equilibrium potential, Nernst equation, over potential & its different types, equilibrium exchange current density- Derivation of Butler Volmer equation-High field & low field approximations

**UNIT IV:**

Charge transfer resistance & polarizability of the interface – concepts of rate determining step, stoichiometric number, reaction order- Determination of step wise mechanism of an electrode reaction- Electro kinetic Phenomena- basic concepts.

**UNIT V: Electro catalysis**

Chemical analysis & Electro catalysis- comparison of Electro catalysis-Electro analysis in simple redox reactions involving adsorbed species-special features of electro catalysis-Discussion on the mechanisms of hydrogen evolution and oxygen reduction reactions.

**Text Book:**

1. D.R. Crow, Principles and Applications of Electrochemistry, Edition – IV, London, Blackie Academic and Professional, 1994

**Reference Book:**

1. S.Glasstone The fundamentals of Electrochemistry.
2. Paul Delahay, Double layer structure and Electrode Kinetics.

**CH314 ELECTRO ANALYTICAL CHEMISTRY****Credits: 3:0:0****Marks : 40 + 60****Unit I:**

Determination of kinetics parameters [  $i_0$ ,  $k_s$ ,  $\beta(\alpha)$ ] by Tafel and linear polarization methods. Ion selective electrodes –selectivity coefficient– amperometric sensing and determination of dissolved oxygen.

**Unit II:**

Linear sweep voltammetry and cyclic voltammetry Derivation of Randles- Sevciks equation –effect of sweep rate-Discussion of reversibility and interpretation of experimental data.

**Unit III:**

Potential step method (chronoamperometry) under diffusion control Derivation of Coettrell equation for a planar and spherical electrode- significance of spherical diffusion – Derivation of Ilkovic equation.

**Unit IV:**

General theory of controlled current methods-Derivation of Sands equation for constant current input under linear diffusion-chrono potentiogram and its significance.

**Unit V:**

Alternating current methods-concepts of Faradaic impedance –derivation of kinetic parameters from impedance measurements – Nyquist and bode plots for simple redox reactions.

**Text Book:**

1. Joseph Wang, Analytical Electrochemistry, II Edition, A. John Wiley & Sons Inc, 2000

**Reference Books:**

1. Paul Delahay, Double Layer Structure and Electrode Kinetics
2. James A. Plam Beck, Electroanalytical Chemistry – Basic Principles and Applications (John Wiley & sons)
3. B.H.Vassos and G.W. Ewing, Electroanalytical Chemistry (John Wiley & sons)

## CH315 MATERIALS ELECTROCHEMISTRY

Credits: 3:0:0

Marks : 40 + 60

### Unit I:

Properties of Spinel-Type Oxide Electrodes: Crystalline Structure and Preparation, Chemical and Electrochemical Parameters, Chemical, Electrochemical and Adsorption Properties,

### Unit II:

Properties of Conductive Transition Metal Oxides with Rutile-Type Structure; Physicochemical Properties of Transition Metal Dioxides, Single Crystals, Mixed Oxide Films.

### Unit III:

Electrochemical Properties of Transition Metal Dioxides, Surface and Intrinsic Redox Properties, Adsorption Properties, electrodic Behavior, Interface: Properties of Oxide Surfaces, adsorption at Gas / Solid Surfaces, Surface Porosity, The Solid / Solution Interface, The Electrical Double Layer at the Oxide / Aqueous Solution Interface,

### Unit IV:

Reactions of Hydrogen and Organic Substances with and at Anodic Oxide Films at Electrodes: Organic Oxidations with Pt and  $\text{PbO}_2$  Anodes, Surface Oxidation of Pt, Mechanisms in Oxidation of  $\text{H}_2$  and Organics,

### Unit V:

Difunctional Mechanism Involving Reactive Surface Oxide, Carbonium-ion Mechanisms, Anodic Reactions of  $\text{H}_2$  and Simple Organic Substances at Catalytic Electrode Surfaces, Oxygen and Chlorine Evolution at Conductive Metallic Oxide Anodes: Concepts in Electrocatalysis.

### Text Book

1. Sergio Trasatti, "Electrodes of Conductive Metallic Oxides", Elsevier Scientific Publishing Company, Amsterdam-Oxford- NY 1980.

### Reference Book

1. Paul Delahay, Double Layer Structure and Electrode Kinetics

## CH316 ELECTRO DEPOSITION TECHNIQUES

Credits: 3:0:0

Marks : 40 + 60

### Unit I:

Formation of simple and complex ions – Ions in solutions of electrolytes – Conductivity of solutions – Quantity of electricity and Faraday's laws – Current efficiency

### Unit II:

Ionization of water – Significance of pH – Determination of pH values by electrometric methods – Theory of pH indicators – Buffer solutions

**Unit III:**

Reversible electrode potential – Its significance - Standard electrode potential and their applications – Electrode potentials and the displacement of metals – Deposition potentials of metals

**Unit IV:**

Hydrogen overvoltage and its importance in metal deposition – Concentration polarization and the diffusion layer – Electrolysis of complex cyanide solutions – Conditions affecting the form of electrodeposited metals – The behaviour of anodes (passivity)

**Unit V:**

Electrodeposition of copper, nickel, chromium, nickel-chromium, zinc, Alloy deposition – Bath formulation – Process sequence – Deposit analysis – Adhesion, Thickness, Porosity, Hardness, Corrosion resistance – Structural and morphological analysis.

**Text book:**

1. E. Raub and K. Muller, Fundamentals of Metal Deposition, ECS Princeton

**Reference Books:**

1. N.V.Parthasarathy, Practical Electroplating Handbook, prentice Hall, Englewood Cliffs, NJ,1989.
2. The Fundamentals of electrochemistry and electrodeposition by S.Glasstone D.Sc.,Ph.D.

**CH317 CHEMISTRY OF ENERGY SOURCES AND STORAGE DEVICES****Credit :3:0:0****Marks : 40+60****Unit I: Chemical Energy Sources**

Introduction to energy; Fuels – Definition, Classification: Natural and synthetic or (i) Primary – Solid, Liquid and Gaseous fuels and (ii) Secondary – Solid, Liquid and gaseous fuels. Importance of hydrocarbons as fuels. Calorific value – definition, classification – Gross and Net calorific values, units (S.I.). Experimental determination of calorific value of solid / liquid fuels by using Bomb Calorimeter, numerical problems. Petroleum cracking – definition, Fluidized bed catalytic cracking. Reforming of petrol – explanation with reactions. Octane Number, Cetane Number. Knocking – mechanism, prevention of knocking – anti-knocking agents, Unleaded petrol. Synthetic petrol – Bergius process and Fischer Tropsch process. Power alcohol.

**Unit II: Electrochemical Energy Storage Devices**

Batteries – Introduction, Basic concepts – principal components of a battery operation of a battery during discharge and charge. Classification of batteries – Primary, Secondary and Reserve batteries with examples. Fuel Cells – Introduction, definition, differences between a battery and a Fuel Cell and advantages. Types of fuel cells – Alkaline fuel cells, Solid polymer electrolyte membrane fuel cells.

### **Unit III: Advanced Non-Conventional Energy Sources - I**

Solar Energy - Photovoltaic cells – Introduction, definition, importance. Solar grade silicon. Properties of silicon relevant to photovoltaics, production of solar grade silicon by chemical vapour deposition method and purification by zone reforming. Doping of silicon and working of a PV cell- Tidal Energy– basic principles; tidal power generation systems; advantages and limitations of tidal power generation.

### **Unit IV: Advanced Non-Conventional Energy Sources - II**

Wind Energy– basic principles of wind energy conversion; advantages and limitations of wind power generation

Geothermal Energy – Origin and nature of geothermal energy; classification of geothermal resources; advantages and limitations of geothermal power generation

Hydrogen Energy - Production of hydrogen from nonrenewable and renewable primary energy forms - Use of hydrogen as an energy carrier.

### **Unit V: Bio Energy and their Advantages**

Biomass and bio-fuels; energy plantation; biogas generation; types of biogas plants; applications of biogas; energy from wastes – Bio-fuels: Types of Bio-fuels - Bio- Ethanol and Bio – Diesel, Production processes and technologies, Bio-fuel applications, Government Policy and Status of Bio fuel technologies in India

### **Reference Books:**

1. John W Twidell and Antony D Weir, 'Renewable energy resources', English Language Book Society (ELBS), 1996
2. Godfrey Boyle, 'Renewable energy – power for sustainable future', Oxford University Press in association with the Open University, 1996
3. S A Abbasi and Naseema Abbasi, "Renewable energy sources and their environmental impact", Prentice Hall of India, 2001
4. G D Rai, 'Non-conventional sources of energy, Khanna Publishers, 2000
5. G D Rai, 'solar energy utilization', , Khanna Publishers, 2000
6. S L sah, 'Renewable and novel energy sources', M I Publications, 1995
7. S Rao and B B Parulekar, "Energy Technology", Khanna Publishers, 1999
8. W.R.Corriss, 'Direct Energy Conversion' :
9. B.V.Desai, 'Alternative Liquid fuels'
10. J C Kuriakose, and J Rajaram, "Chemistry in Engineering and Technology", Tata Meraw-Hill Publications Co. Ltd., New Delhi, 1996
11. Leo J. M. J. Blomen, Michael N. Mugerwa, 'Fuel Cell Systems' Springer publishers
12. Clive DS Tuch – Modern Battery Technology, Ellis Harwood, New York, 1991.

## **CH318 ORGANIC CHEMISTRY**

**Credit :3:0:0**

**Marks : 40+60**

### **Unit I: Reaction Mechanism –I**

Effect of structure and reactivity – Resonance and field effects –Steric effects- Quantitative treatments of the effect of structure and reactivity –LFER- Hammett and Taft equation

Aromaticity – Huckel's rule – Aromatic systems with electron numbers other than six-annulenes and heteroannulenes – chemistry of fullerenes – Aliphatic nucleophilic substitution

–mechanisms –  $S_N^2$ ,  $S_N^1$ , mixed,  $S_N^1$  &  $S_N^2$ ,  $S_N^i$ . SET, neighbouring group mechanism – Reactivity – effect of substrate, attacking nucleophile, leaving group and reaction medium – substitution at vinylic and allylic carbons.

Aromatic nucleophilic substitutions – mechanisms –  $S_N^Ar$ ,  $S_N^1$ , Benzyne – reactivity – effect of substrate, leaving group and attacking nucleophile

## Unit II: Electrophilic Substitution Reaction

Aliphatic electrophilic substitution – Arenium ion mechanism – Orientation and reactivity in monosubstituted benzene rings – benzene rings with more than one substituent – effect of leaving group – o/p ratio

Addition to C=C – multiple bonds – mechanisms – electrophilic, nucleophilic, free radical – orientation and reactivity – addition of conjugated systems.

Elimination – mechanisms of  $\beta$  elimination – ( $E_2$ ,  $E_1$ ,  $E_{1CB}$ )

orientation of double bonds – reactivity – effect of substrate, attacking base, leaving group and medium.

## Unit III: Stereochemistry

Stereoisomerism – definitions and classification – molecular representation and inter conversion – introduction to molecular symmetry and point groups with examples – Conformation analysis – cyclic system – cyclohexane – conformation and reactivity with examples from molecular rearrangements

Stereoselectivity – classification, terminology, principle of stereoselectivity, example of diastereoselectivity and enantioselectivity including few examples from pericyclic reactions – circular dichroism – ORD – Cotton effect – application of ORD.

## Unit IV: Reagents In Organic Synthesis

Use of the following reagents in organic synthesis and functional group transformations – complex metal hydrides, Gilman's reagent, lithium dimethyl cuprate, lithium diisopropyl amide (LDA), dicyclohexyl carbodiimide, 1,3-dithiane, Woodward and Prevost hydroxylation, DDQ, selenium dioxide, crown ethers and Peterson's synthesis, Wilkinson's catalyst, Baker yeast

## Unit V: Heterocyclics and Supramolecules

Heterocyclics – Nomenclature – compounds containing two hetero atoms – azoles – chemistry of pyrazole, imidazole, oxazole, isoxazole, thiazole and isothiazole – diazines – pyrimidines

Supramolecular chemistry – preparation and structure of catenanes and rotaxanes – molecular recognition – synthetic applications of calixarenes and cyclodextrins – organic reactions on solid supports zeolite, clay, alumina and silica

### Text Books

1. Peter Sykes, Principles of Organic Reaction Mechanism (for 1 – 3 units)
2. Morrison and Boyd, Text Book of Organic Chemistry (for 4 – 5 units)

### Reference Books

1. Jerry March "Advanced Organic Chemistry", Wiley Eastern Limited, Fourth edition, New Delhi, 1999.
2. Rai K. Bansal, "Organic reaction mechanism" Tata McGraw Hill, New Delhi, 1990.

3. F.A.Cary, "Organic chemistry" second edition, McGrawHill, Inc., 1992.
4. P.S.Kalsi, "Stererochemistry", Wiley Eastern Limited, New Delhi, 1990.
5. R.O.C.Norman, "Principles of organic synthesis" second edition, Chapman and Hall, London, Newyork, 1978.
6. V.K.Ahluwalia and Ram Agarwal, "Organic synthesis", Narosa Publishing House, NewDelhi.
7. I.L.Finar, "Organic chemistry" Vol I, ELBS, fifth edition, 1989.
8. R.K.Bansal, "Heterocyclic Chemistry", Wiley eastern, 1990.

### **CH319 RESEARCH METHODOLOGY IN CHEMISTRY**

**Credit :3:0:0**

**Marks : 40+60**

#### **Unit I: Types of Research**

What is research - starting your own research – the research problem- some common mistakes- Aids to locating and analyzing problems.

Information- finding the information –sources of information –dealing with information – reading –note taking –conclusions

Types of Research- historical-comparitive-descriptive-correlation-experimental-evaluation-action-ethnogenic-feminist-cultural

#### **Unit II: Data Analysis**

Errors in chemical analysis – classification of errors-determination of accuracy of methods-improving accuracy of analysis-significant figures – mean standard deviation – comparison of results . "t" test, "f" test and "chi" square test –rejection of results –presentation of data.

Sampling: introduction – definitins – theory of sampling- stastical criteria of good sampling and required size – stratified sampling vs random sampling –minimistion of varience in stratified sampling – transmission and storage of samples.

#### **Unit III: Chromatography**

Gas Chromatography- Theory of chromatography-column efficiency and column equation-sample injection-sampling system for capillary column and packed column-detectors –gas flow control system – HPLC principles of HPLC –the liquid chromatograph-the requirements of solvent pumping and different pumping system, gradient elution, isocratic elution. – detectors and column selection for HPLC

#### **Unit IV: Separation Techniques**

Separation by precipitation –separation by solvent extraction-theory & application of solvent extraction – Chromatography- classification and principles of column chromatography-ion exchange chromatography – paper chromatography – thin layer chromatography.

Purification techniques

Purification techniques for solids- crystallitation- fractional crystalitation- sublimation-solvent extraction

purification techniques for liquids-simple distillation-fractional distillation-distillation under reduced pressure-steam distillation.

### **Unit V: Instrumentation**

Thermo analytical methods- TG- characteristic features of thermogram –instrumentation of thermogravimetry –factors affecting TGA- applications of TGA.

DTA- characteristic of DTA curves –instrumentation of DTA –factors affecting DTA applications of DTA.

XRD- a brief account of the principles of molecular structure determination by X-ray diffraction by single crystal-structure factor-.

### **Reference Books:**

1. Nicholas Walliman "Your research project" - SAGE publication.2001.
2. S.Usharani," Analytical Chemistry", first edition, Mcmillan,India ltd, 2000.
3. Williar,Merritt and Dean ,"Instrumental Methods of Analysis", sixth edition, Williard H.H., 1991.
4. Douglas A.Scoog ,Donald M.West and F.James Holler ,"Analytical chemistry and introduction", Saunders,College publishing,Newyork,1992.

## ADDITIONAL SUBJECTS

| <b>Code No.</b> | <b>Subject</b>                                  | <b>Credits</b> |
|-----------------|---|----------------|
| CH107           | Chemistry for Civil Engineers                   | 3:0:0          |
| CH108           | Chemistry for Mechanical Engineers              | 3:0:0          |
| CH109           | Chemistry for Electrical and Computer Engineers | 3:0:0          |
| CH110           | Principles of Organic Chemistry                 | 3:0:0          |
| CH201           | Environmental Science and Engineering           | 3:0:0          |
| CH320           | Physical Chemistry – I                          | 4:0:0          |
| CH321           | Organic Chemistry – I                           | 4:0:0          |
| CH322           | Inorganic Chemistry – I                         | 4:0:0          |
| CH323           | Inorganic Chemistry Lab                         | 0:0:4          |
| CH324           | Industrial Chemistry                            | 4:0:0          |
| CH326           | Analytical Chemistry – I                        | 4:0:0          |
| CH327           | Physical Chemistry – II                         | 4:0:0          |
| CH328           | Organic Chemistry – II                          | 4:0:0          |
| CH329           | Inorganic Chemistry – II                        | 4:0:0          |
| CH330           | Organic Chemistry Lab                           | 0:0:4          |
| CH331           | Solid State Chemistry                           | 4:0:0          |
| CH332           | Analytical Chemistry – II                       | 4:0:0          |
| CH333           | Physical Chemistry – III                        | 4:0:0          |
| CH334           | Organic Chemistry – III                         | 4:0:0          |
| CH335           | Inorganic Chemistry – III                       | 4:0:0          |
| CH336           | Physical Chemistry Lab                          | 0:0:4          |
| CH337           | Environmental Chemistry                         | 4:0:0          |
| CH338           | Petroleum Chemistry                             | 4:0:0          |
| CH339           | Advanced Pharmaceutical Chemistry               | 4:0:0          |
| CH340           | Industrial Electrochemistry                     | 4:0:0          |
| CH341           | Biochemistry                                    | 4:0:0          |
| CH342           | Polymer Chemistry                               | 4:0:0          |
| CH343           | Instrumental Methods of Analysis                | 4:0:0          |
| CH344           | Natural Products Chemistry                      | 4:0:0          |
| CH345           | Chemistry of Dyes and Pigments                  | 4:0:0          |
| CH346           | Textile Processing                              | 4:0:0          |
| CH347           | Chemistry and Processing of Electroceramics     | 4:0:0          |
| CH348           | Advanced Spectroscopy                           | 4:0:0          |
| CH349           | Medicinal Chemistry                             | 4:0:0          |
| CH350           | Nanochemistry                                   | 4:0:0          |
| CH351           | Green Chemistry                                 | 4:0:0          |
| CH352           | Recent Advances in Chemistry                    | 4:0:0          |
| CH353           | Supramolecular Chemistry                        | 4:0:0          |
| CH354           | Corrosion Science and Engineering               | 4:0:0          |

**CH107 CHEMISTRY FOR CIVIL ENGINEERS**  
**(For B.Tech Civil – Semester I / II)**

**Credits:3:0:0**

**Unit I: Polymers and Composites**

Basic concepts – polymerization – plastics – thermoplastics and thermosetting plastics – Engineering plastics – Miscellaneous polymers - Composite materials – Application of composites – Constituents of Composites – Types of Composites – Fibre reinforced composites – Types – Particulate composites – Types - Layered composites – Processing of fibre reinforced composites

**Unit II: Water Testing & Sewage Treatment**

Testing of water for the following parameters – pH – Total dissolved solids (TDS) – Total suspended solids (TSS) – Acidity – Alkalinity – Hardness – Determination of Ca, Magnesium, Sodium, Potassium, Iron, Sulphate, Chloride, Fluoride, Phosphate and Silica content – Determination of BOD and COD – Sewage – Constituents of sewage – Aerobic and Anaerobic oxidation – Sewage treatment – Preliminary process – Settling process – Biological (or secondary) treatment process – Tertiary treatment

**Unit III: Inorganic Building Materials:**

Cement – Classification. Portland cement - chemical composition-manufacture, reactions during setting and hardening physical properties, ISI specifications of Portland cement. Decay of cement – prevention. Lime – setting, plaster of Paris – setting and hardening, applications. Porcelain – properties and applications.

**Unit IV: Corrosion and control:**

Corrosion losses, chemical corrosion- oxidation, pilling - bedworth rule. electrochemical corrosion - galvanic corrosion, differential aeration corrosion-pitting corrosion, water line corrosion, stress corrosion, soil corrosion, atmospheric corrosion. Factors influencing corrosion. Corrosion of concrete – monitoring methods. Corrosion control – cathodic protection, selection of materials and proper designing, use of corrosion inhibitors.

**Unit V: Coatings and Adhesives**

Coating – organic coatings - paints – constituents and their functions, mechanism of drying. Formulation of paints, failure of paint films, varnishes lacquers and enamels. Special paints – fire retardants, water repellent, temperature indicating and luminous paints. Adhesive bonding- adhesive action, development of adhesive strength- physical and chemical factors influencing adhesive strength.

**Text Books**

1. Jain P C and Monica Jain, "Engineering Chemistry", Dhanpat Rai Publishing Company (P) Ltd., New Delhi, 2006.
2. Shashi Chawla, "A Text book of Engineering Chemistry", Dhanpat Rai Publishing Company (P) Ltd., New Delhi, 2007.
3. S. S. Dara, A Text book of Engineering Chemistry I and II", 4<sup>th</sup> revised edition, S. Chand and Co.1994
4. N. Manivasakam, "Physico-chemical Examination of Water Sewage and Industrial Effluents", Pragati Prakashan, 1996

**CH108 CHEMISTRY FOR MECHANICAL ENGINEERS**  
**(For B.Tech Mechanical Semester I / II)**

**Credits:3:0:0**

**Unit I: Polymers and Composites**

Basic concepts – polymerization – plastics – thermoplastics and thermosetting plastics – Engineering plastics – Miscellaneous polymers - Composite materials – Application of composites – Constituents of Composites – Types of Composites – Fibre reinforced composites – Types – Particulate composites – Types - Layered composites – Processing of fibre reinforced composites

**Unit II: Dynamics of Chemical Process**

Rate of reaction – Determination of rate of reaction – Expression of reaction rates – Factors influencing reaction rates – Order of a reaction – Molecularity – Derivation of kinetic equations – (first order and second order) – Collision theory – Activation energy and Arrhenius equation – Derivation of Arrhenius equation - Complex reactions – Opposing reaction, Consecutive reactions, parallel or competing reactions, Branched chain reactions leading to explosion and chain reactions – (Explanations with example and no derivations for complex reactions) – Catalysis – Michaelis – Menton equation – Derivation

**Unit III: Fuels and Combustion**

Calorific value - gross and net calorific values - Proximate and ultimate analyses of coal – Significances – Characteristics of metallurgical coke – manufacture by Otto – Hoffman method – Synthetic petrol – Bergius process – Fischer – Tropsch's process – Knocking – Octane number – Improvement of anti knocking characteristics – Cetane number, gaseous fuels – composition and manufacture of Water gas, producer gas - CNG (definition only) – Flue gas analysis – Orsat's apparatus.

**Unit IV: Lubricants and Adhesives**

Lubricants – Classification, Mechanism of lubrication, lubricating oils, semi solid lubricants (greases), solid lubricants, synthetic lubricants, testing of lubricating oils - viscosity index, flash and fire point, cloud and pour point, aniline point, steam emulsion number, carbon residue, neutralization number and other properties.

Adhesive bonding - adhesive action, Development of adhesive strength - physical and chemical factors influencing adhesive strength.

**Unit V: Corrosion and Control**

Corrosion losses, chemical corrosion- oxidation, Pilling-Bedworth rule, electrochemical corrosion - galvanic corrosion, differential aeration corrosion-pitting corrosion, water line corrosion, stress corrosion soil corrosion, atmospheric corrosion, Factors influencing corrosion, Corrosion control – cathodic protection , selection of materials and proper designing, use of corrosion inhibitors.

**Text Books**

1. Jain P C and Monica Jain, "Engineering Chemistry", Dhanpat Rai Publishing Company (P) Ltd., New Delhi, 2006.

2. Shashi Chawla, "A Text book of Engineering Chemistry", Dhanpat Rai Publishing Company (P) Ltd., New Delhi, 2007.
3. S. S. Dara, "A Text book of Engineering Chemistry I and II", 4<sup>th</sup> revised edition, S. Chand and Co. 1994

**CH109 CHEMISTRY FOR ELECTRICAL AND COMPUTER ENGINEERS**  
**(For B.Tech - ECE/EEE/E& I/CSE/IT/E&MT – Semester I / II)**

**Credits:3:0:0**

**Unit I: Engineering Materials & Applications**

Introduction – Superconductors – Types – Properties of superconductors – Applications of superconductors – Properties – Preparation of the 1:2:3 or  $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$  superconductor – Optical fibres – Organic Electronic Materials

**Unit II: Nanopowders and Nanomaterials**

Preparation – Chemical Vapour Deposition – Sol-gels process – Electrodeposition – Natural nanoparticles – Application of nano-particles – Insulation materials – Machine tools – Phosphors – Medicinal implants

**Unit III: Electrochemistry and Corrosion**

Origin of potential – electrical double layer – reversible electrode potential – standard hydrogen electrode – electro motive series – measurement of potential – reference electrodes (calomel and silver/silver chloride) indicator and ion selective electrodes – Nernst equation – irreversible processes – over potential - Corrosion - electrochemical corrosion - galvanic corrosion, differential aeration corrosion, stress corrosion - Factors influencing corrosion - Corrosion control – cathodic protection, selection of materials and proper designing, use of corrosion inhibitors.

**Unit IV: Electrochemical Power Sources**

Batteries – primary and secondary – dry cell, alkaline, Ni-Cd battery, mercury battery, lead-acid battery, solar battery, Ni- Metal hydride battery, activated batteries (sea water activated batteries) Fuel cells – Types – Low temperature, medium temperature and high temperature fuel cells.

**Unit V: Advanced Electronic Materials**

Carbon nanotubes (CNT) – Use of CNT in electronics - Fullerenes – Polymer nano-composites – Shape memory alloys – Metallic glasses - solid oxide materials  
Fundamental of semiconductor Technology – Semiconductor materials – Chemistry of Fabrication steps– Single crystal Growth – Photolithography – Etching – Metallization

**Text Books**

1. Jain P C and Monica Jain, "Engineering Chemistry", Dhanpat Rai Publishing Company (P) Ltd., New Delhi, 2006.
2. Shashi Chawla, "A Text book of Engineering Chemistry", Dhanpat Rai Publishing Company (P) Ltd., New Delhi, 2007.

3. Garry S. May and Simon M. Sze, "Fundamentals of Semiconductor Fabrication" John Wiley & Sons, Inc, 2004
4. Michael Wilson, Kamali Kannangara, Geoff Smith, Michelle Simmons and Burkhard Raguse, "Nanotechnology – Basic Science and Emerging Technologies", Chapman & Hall (CRC), 2004

**CH110 PRINCIPLES OF ORGANIC CHEMISTRY**  
**(For B.Tech. - BioTech / BioInfo / Food Processing – Free Elective)**

**Credits:3:0:0**

**Unit I: Structure of Organic Compounds**

Nature of bonds – covalent bond, geometry of molecules, hybridization, bond length, polarity of bonds, inductive effect, electromeric effect, resonance, delocalization, hyper conjugation, acids and bases.

**Unit II: Nature of Organic Reactions**

Types of organic reactions - Heterolytic reactions, Carbocations – stability, formation and reactions, Ionic mechanism – substitution – nucleophilic, electrophilic, elimination – E<sub>1</sub>, E<sub>2</sub>. Addition – nucleophilic, electrophilic, Molecular rearrangement, Polymerization, Free radicals – formation, stability and reactions.

**Unit III: Introduction to Stereochemistry**

Isomerism – Types – structural isomerism– resonance, Conformational isomers – Newmann projection formula. Stereoisomerism – geo-isomers – nomenclature, properties. Optical isomerism – plane of symmetry, centre of symmetry, optical isomers of lactic acid, R & S notation, Resolution – methods.

**Unit IV: Chemistry of Proteins**

Composition of proteins – nature – classification – isolation - chemical properties, Analytical tests - estimation of free amino groups and carboxyl groups, Uses of proteins.

**Unit V: Medicinal Chemistry**

Antibiotics – streptomycin, tetracycline, chloroamphenicol, Antimalarial – derivatives of 4-aminoquinoline, Antipyretics – aspirin, analgin, paracetamol, Definition and examples for analgesics, hypnotics, tranquillizers.

**Text Books**

1. P.L.Soni, Text book of Organic Chemistry, SultaN Chand and sons, 28<sup>th</sup> edition, New Delhi, 1999.
2. Morrison and Boid, "Organic Chemistry", 3<sup>rd</sup> edition, United states of America, 1980
3. B. S. Bahl and Arun Bahl, "Text book of Organic Chemistry", New Delhi, S. Chand & company Ltd., 1994

## CH201 ENVIRONMENTAL SCIENCE AND ENGINEERING

**Credit 3:0:0**

### **Unit I - Natural resources, ecosystems and biodiversity**

Environment - Definition, scope and importance – Forest resources: Use and overexploitation, Water resources: Use and over-utilization, dams-benefits and problems – Energy resources: Growing energy needs, renewable and non renewable energy sources, use of alternate energy sources – Land resources: land degradation – Role of an individual in conservation of natural resources Ecosystem – Structure and function – Ecological succession – Introduction to various ecosystems. Biodiversity – Definition and types – Threats to Biodiversity in India and its impacts – Conservation of Biodiversity: In-situ and Ex-situ conservation of biodiversity

### **Unit II – Air pollution and global issues**

Air pollution - Introduction – atmospheric constituents – Chemical reaction in the atmosphere – air pollutants – classification – effects on human, animal, plant, property and environment – control methods for particulates and gaseous pollutants – control of pollutants from automobiles – Burning of plastics – PCBs and their impact - Green house gases – green house effects - climate change - global warming and its effects – international climate conventions, protocols and perspectives – technology and policy options for GHG emission mitigation - acid rain, ozone layer depletion and solutions

### **Unit III – Water and other environmental pollutions**

Water pollution - sources – characteristics – BOD, COD - pollutants and their effects – heavy metal pollution – inorganic and organic pollutants control methods – screening, sedimentation, biological processes - working and design principles – advanced waste water treatment techniques - self purification of rivers – eutrophication of lakes – sludge management  
Soil pollution - marine pollution - noise pollution - thermal pollution - nuclear hazards - Causes, effects and control measures - solid waste management: causes, effects and control measures of urban and industrial solid wastes

### **Unit IV – Environmental Legislation**

Pollution controls acts – environment protection act – water pollution act – air pollution act – wildlife (protection) act, 1972 – forest (conservation) act, 1980 – polluter pays principle – precautionary principle – Issues in pollution control enforcement and public awareness – issues of environment – public awareness

### **Unit V - social issues and the environment**

From Unsustainable to Sustainable development – Urban problems related to energy – Water conservation, rain water harvesting, watershed management - Population growth, variation among nations – Population explosion - Environment and human health – Role of Information Technology in Environment and human health - Disaster management: floods, earthquake, cyclone and landslides

**Text books:**

1. Deswal S and Deswal A, 'A basic course in Environmental studies', Dhanpat Rai & Co, First edition, Delhi, 2004
2. Kurian Joseph and Nagendran R, 'Essentials of Environmental studies', Pearson Education Pvt Ltd., First edition, Delhi, 2004
3. Santhosh Kumar Garg, Rajeswari Garg and Ranjani Garg, 'Environmental Science and Ecological Studies', Khanna Publishers, Second Edition, New Delhi, 2007.

**Reference books:**

1. Gilbert M.Masters, 'Introduction to Environmental Engineering and Science', Pearson Education Pvt. Ltd., Second Edition, 2004.
2. Tivedi R.K., 'Handbook of Environmental Laws, Rules, Guidelines, Compliances and Standards, Vol. I and II, Enviro Media., 1998
3. Cunningham, W.P.Cooper, T.H.Gorhani, 'Environmental Encyclopedia', Jaico Publ., House, Mumbai, 2001.
4. Wager K.D., 'Environmental Management,' W.B. Saunders Co., Philadelphia, USA, 1998.

**CH320 PHYSICAL CHEMISTRY - I****Credits:4:0:0****Unit I : Chemical thermodynamics – I**

The First Law of Thermodynamics - Work, heat, and energy - State functions and reversible processes - Enthalpy and applications to chemical reactions - The Second Law of Thermodynamics - Entropy and spontaneous processes - Entropy and disorder - The Third Law of Thermodynamics – entropy at absolute zero – Trouton's rule - calculation of entropy - *Helmholtz* and Gibbs Energies - the meaning of free energies - Maxwell relations

**Unit II : Chemical thermodynamics – II**

The standard state and calculation of thermodynamic functions - Fugacity: *nonideal* behavior of gases - Phase *Equilibria* - Chemical potential and the Gibbs phase rule - Typical phase diagrams - *Clausius-Clapeyron* relation - Solutions - Partial molar properties - Gibbs-*Duhem* equation - Ideal solution and activity of real solutions - Chemical Equilibrium - Application of thermodynamics to chemical reactions - Equilibrium constants and their calculation

**Unit III : Statistical thermodynamics – I**

Concepts of probability and Maxwell Boltzmann distribution – Basic derivation – prove that  $B = 1/KT$  – Relationship between entropy and thermodynamic probability systems with degeneracy – Definitions of partition function – applications – derivation of thermodynamic functions from partition function – entropy for monoatomic gases – Sackur – Terode equation – The Bose – Einstein's system – Basic derivation – Fermi – Dirac system – Basic derivation – negative Kelvin temperature

#### **Unit IV : Statistical thermodynamics – II**

Heat capacity of solids – Debye and Einstein models – Thermodynamics functions of ideal gases, translational, vibrational and rotational contributions at different levels of approximation

Irreversible thermodynamics – the steady – coupled flows – application – over potential – decomposition potential – electrical double layer and electro kinetic phenomena – structure of electrical double layer – capacity – E.K. phenomenon – steaming potential – electro dialysis – the Dom effect

#### **Unit V : Phase rule**

Phase rule and phase equilibria – one and two components – overview – Iron, carbon equilibrium diagram – Interpretation – allotropy – heat treatment – three component system – graphical representation systems with two salts and water.

#### **Text books:**

1. B.R., Puri, L.R. Sharma and Madan S. Pathania, “Principles of Physical Chemistry”, Shoban Lal Nagin Chand & Co., Jalandhar, 2000.
2. Kundu and S.K. Jain, “Physical Chemistry” S. Chand & Company Ltd., New Delhi, 1984
3. P.W. Atkins, “Physical Chemistry”, 5<sup>th</sup> edition, Oxford University Press, 1995

#### **Reference Books:**

1. S. Glasstone and D.Lewis, “Elements of Physical Chemistry”, 2nd Ed.,1982
2. N.D. Smith, “Elementary Statistical Thermodynamics”, Plenum Press, New York, 1982
3. M.J. Piling and P.W. Seakins, “Reaction Kinetics”, Oxford University Press, 2<sup>nd</sup> edition, 1996
4. J. C. Kuriacose and J.Rajaram, “Thermodynamics”, Shoban Lal Nagin Chand & Co., Jalandhur, 1996
5. S Glasstone, “Thermodynamics for Chemists”, Affiliated West Wes Press, New Delhi, 1965
4. B.C. McClelland, “Statistical Thermodynamics”, Chapman and Hall, London, 1973
5. M. C. Gupta, “Statistical Thermodynamics”, Wiley Eastern Limited, 1993
6. L.K. Nash, “Elements of classical the statistical thermodynamics”, Addison-Wesley (1970)
7. 1996
8. G.W. Castellan, “Physical Chemistry”, Narosa publishing house, Chennai, 1989
9. H. Snehe, “Comprehensive Physical Chemistry”, Prgati Prakashan, Meerut, 1987

### **CH321 ORGANIC CHEMISTRY - I**

**Credits:4:0:0**

#### **Unit I : Stereochemistry – I**

Stereoisomerism – definitions and classification – molecular representation and inter conversion – Classification of stereo isomers – Stereoisomerism and center of chirality – molecules with a single stereogenic center – configurational nomenclature – molecules with

two or more chiral centers – Stereoisomerism in cyclic compounds – axial chirality, planar chirality and helicity principles of axial principles of axial and planar chirality – molecules with axial chirality

### **Unit II : Stereochemistry – II**

Topivity and pro stereo isomerism – Homotopic ligands and faces – enantio topic ligands and faces – diastereotopic ligands and faces, Nomenclature of stereoheterotopic ligands and faces. Molecules with one prochiral centre – Re and Si system of nomenclature for ligands – principles of stereoselectivity – Substrate selectivity – product selectivity – asymmetric synthesis – Cram and Prelog's rule – biochemical asymmetric transformations – catalytic nexus – confirmations of typical and atypical examples of substituted cyclohexanes and decalins, Klyne – Prelog nomenclature of conformation.

### **Unit III : Reaction Mechanism – I**

Effect of structure and reactivity – Resonance and field effects – Steric effects – Quantitative treatments of the effect of structure and reactivity – LFER – Hammett and Taft equation – Importance of  $\sigma$  and  $\rho$  values in aromatic electrophilic substitutions – Labelling and kinetic isotopic effects.

Aromaticity – Huckel's rule – Aromatic systems with electron numbers other than six – annulenes and hetero annulenes – Chemistry of fullerenes.

### **Unit IV : Reaction Mechanism – II**

Aliphatic nucleophilic substitution – mechanisms –  $S_N^2$ ,  $S_N^1$ , mixed  $S_N^1$  and  $S_N^2$ ,  $S_N^i$ , SET, neighbouring group mechanism – Reactivity – effect of substrate, attacking nucleophile, leaving group and reaction medium – Substitution at vinylic and allylic carbons.

Aromatic nucleophilic substitutions – mechanism -  $S_N^{Ar}$  -  $S_N^1$  – Benzyne – reactivity – effect of substrate, leaving group and attacking nucleophile.

### **Unit V : Reaction Mechanism – III**

Aromatic electrophilic substitution – Arenium ion mechanism – Orientation and reactivity in monosubstituted benzene rings – benzene rings with more than one substituent - effect of leaving group – o/p ratio.

Addition to C-C-multiple bonds – mechanisms – electrophilic, nucleophilic, free radical – orientation and reactivity – addition of conjugated systems

Elimination – mechanisms of  $\beta$  elimination – ( $E_2$ ,  $E_1$ ,  $E_{1CB}$ ) –  $E_1$  –  $E_2$  –  $E_{1CB}$  spectrum, orientation of double bonds – reactivity – effect of substrate, attacking base, leaving group and medium.

### **Text Books:**

1. Jerry March, "Advanced Organic Chemistry", Wiley Eastern Limited, Fourth edition, New Delhi, 1999
2. Morrison and Boyd, "Organic Chemistry", 3<sup>rd</sup> edition, United States of America, 1980
3. B. S. Bahl and Arun Bahl, "Text book of Organic Chemistry", New Delhi, S. Chand & company Ltd., 1994
4. Peter Skyes, "A Guidebook to Mechanism in Organic Chemistry". Longman Press, London and New York, 1995

- Ernest. L. Eliel, "Stereochemistry of carbon compounds", 22<sup>nd</sup> reprint, Tata-McGraw Hill, New Delhi, 1997

**Reference Books:**

- I.L. Finar, "Organic Chemistry, Volume 1: The Fundamental Principles", London Longmans, 1963
- T.W.G. Solomons, "Organic Chemistry", Vol.2, ELBS, 1989
- Indian Journal of Chemistry (A and B), special issues on Fullerenes, Vol. 31 A, A & B, No. 5, March 1992
- Rai K. Bansal, "Organic reaction mechanism", Tata McGraw Hill, New Delhi, 1990
- F.A. Cary, "Organic Chemistry", Second edition, McGraw Hill, Inc., 1992
- P.S. Kalsi, "Stereochemistry", Wiley Eastern Limited, New Delhi, 1990
- D. Nasipuri, "Stereochemistry of organic compounds – Principles and applications" 2<sup>nd</sup> edition, New Age international, 2002
- R. Curl, Accounts of Chemical Research, "Special issue on Buckminster Fullerenes", Vol. 25, No. 3, March 1992, pages 98 - 105

**CH322 INORGANIC CHEMISTRY - I**

**Credits:4:0:0**

**Unit I : Structure and Bonding**

Ionic bond – Formation – Characteristics of ionic compounds, melting point, boiling point, hardness, electrical conductivity, solubility – structure of crystal lattices – Lattice energy; Boron-Lande equation and Born Heber Cycle – Polarisation of ions: Fajan's rule – Calculation of some limiting ratio values – Covalent bond – Rules for covalent bond formation – Valence bond theory – Resonance and hybridization – Molecular orbital theory and its application in diatomic molecules – Comparison of VB and MO theories – The concept of multicentered bond as applied to electron deficient molecules (boron hydrides) – Bond properties – bond energy – bond length – bond polarity - electron pair repulsion theory and its applications – Hydrogen bond – types – effect on molecular properties – detection of hydrogen bonding.

**Unit II : Solids**

Bond theory of solids – Electrical properties – insulators – semi conductors – superconductors – dislocation in solids – Schottky and Frenkel defects – Structure of some compounds of AX, AX<sub>2</sub> and A<sub>m</sub>X<sub>2</sub> types – perovskite, ilmenite and spinel structures

### **Unit III : Nuclear Chemistry**

Modes of radioactive decay and rate of radioactivity decay – Radioactive detectors – types of nuclear reactions – Artificial radioactivity – Nuclear stability – packing fraction – mass defects and binding energy – nuclear fission of uranium, liquid drop model – nuclear fusion – essential features of water coated thermal reactors and fast breeders – neutron activation analysis – carbon and rock dating – applications of tracers in chemical analysis, reaction mechanisms, medicine and industry

### **Unit IV : Chemistry of Non-transition elements**

Polymorphism of carbon, phosphorous and sulphur – synthesis, properties and structure of silicates, carbides, silicones, phosphazenes, sulphur – nitrogen compounds – Interhalogens and pseudohalides – oxyacids of selenium and tellurium

### **Unit V : Chemistry of lanthanides and actinides**

Lanthanides – position in the periodic table – general properties of lanthanides and actinides – electronic configuration, oxidation state and oxidation potential, atomic and ionic radii – Cause and consequences of lanthanide and actinide contractions – comparison of spectral and magnetic properties of lanthanide and actinide complexes – Extraction details of cerium, thorium and uranium – Chemistry of their important compounds: Oxides, nitrates and sulphates

#### **Text Books:**

1. F.A. Cotton and G. Wilkinson, “Advanced Inorganic Chemistry”, 5<sup>th</sup> edition, John Wiley and Sons, New York, 1988
2. James E. Huheey, “Inorganic Chemistry”, 4<sup>th</sup> Edition, Addison Wesley Publishing Company, New York, 1993
3. B.R. Puri and L.R.Sharma, “Principles of Inorganic Chemistry”, Shoban Lal Nagin Chand and Co., 1989
4. J.D. Lee, “Concise Inorganic Chemistry”, 5<sup>th</sup> edition, ELBS with Chapman and Hall, London, 1996

#### **Reference Books:**

1. D.E. Shriver, B.W. Atkins and C.H. Langford, “Inorganic Chemistry” 2<sup>nd</sup> edition, (ELBS), Oxford University press, 1994
2. F.A. Cotton and G. Wilkinson, “Advanced Inorganic Chemistry”, 5<sup>th</sup> edition, John Wiley and Sons, New York, 1988
3. H.J. Arnika, “Essentials of Nuclear Chemistry”, 4<sup>th</sup> Ed., New Age International Publishers Ltd., New Delhi, 1995
4. B.K. Sharma, “Nuclear and Radiation Chemistry” Krishna Prakashan Media Pvt. Ltd., Meerut, 1997

### **CH323 INORGANIC CHEMISTRY LAB (6 hours)**

**Credits:0:0:4**

12 experiments will be notified by the HOD from time to time

### **CH324 INDUSTRIAL CHEMISTRY**

**Credits:4:0:0**

### **Unit I. Cement and Lime**

Manufacture of Portland cement – setting and hardening of Portland cement – regauging cement – effect of fineness on setting and hardening – freezing – high early strength cement – high alumina cement

Lime – raw materials- manufacture – slaking – lime mortar – types of lime – high – calcium or fat lime – calcium lime or lean lime – magnesian lime – dolomitic lime – hydraulic lime.

### **Unit II. Abrasives and Refractories**

Abrasives – hard abrasives – siliceous abrasives – soft abrasives – artificial abrasives - uses

Refractories – definition – classification – acid refractories – basic refractories – neutral refractories – properties - uses

### **Unit III. Inorganic chemicals**

Common salt and soda ash – Manufacture – Different grades – products – alkalis –  $\text{Na}_2\text{CO}_3$   
Caustic soda and chlorine industry – manufacture principles of electrolytic process – chlorine – storage

Hydrochloric acid – manufacture – absorption – uses

Sulphur and sulphuric acid – extraction of sulphur – manufacture of  $\text{H}_2\text{SO}_4$  – chamber – contact processes – industrial uses

### **Unit IV. Explosives**

Explosives – uses – properties and tests – explosives for war – nitrocellulose – picric acid and T.N.T. – industrial explosives – nitroglycerin and dynamites – black powder – smoke screens – incendiaries – gas mask

### **Unit V. Agriculture chemicals**

Fertilizers – organic and inorganic – ammoniated superphosphates, sodium nitrate solid pellets – potassium salts – pesticides – fungicides – herbicides – their preparations and characteristics – environmental impacts.

#### **Text Books:**

1. B.K. Sharma “Industrial Chemistry”, Goel Publishing House, Meerat, 2000
2. S.D. Shukla and G.N. Pandey, “A text book of chemical technology”, Vikas publishing house pvt. Ltd, New Delhi, 1979
3. M. Gopal Rao, “Outline of chemical technology”, Affiliated East – West press Ltd., Chennai, 1973.
4. J.E. Huheey, “Inorganic Chemistry”, Harper & Row publishers, New York, 1972
5. Sathya Prakash, G.D. Tuli, S.K. Basu and T.D. Madan, “Advanced Inorganic Chemistry”, S.Chand & Company, New Delhi, 17<sup>th</sup> edition, 1988

#### **Reference Books:**

1. R.N. Sherve, “Chemical process industries”, McGraw-Hill, Kugakuisha Ltd., Tokyo, 1984
2. Riegels Hand Book of Industrial Chemistry, 9<sup>th</sup> edition, edited by James A. Kent., New York, Van Nostrand Reinhold, 1992

## CH326 ANALYTICAL CHEMISTRY - I

**Credits:4:0:0**

### **Unit I : Errors and the treatment of Analytical Data**

Errors, Types of errors, Minimization of determinate errors: Accuracy and Precision, Distribution of random errors, statistical treatment of finite samples – Measures of central tendency and variability, Student's confidence interval of the mean, testing for significance and criteria for rejection of an observation, control charts, propagation of errors, significant figures and computation rules, Correlation coefficient, method of least squares.

### **Unit II : Theory of volumetric and gravimetric analysis**

Acid base titrations – classification – theory of acid – based titration – neutralization – indicators – neutralization curves – choice of indicators in neutralization reaction

Gravimetric analysis – theory of gravimetric analysis – solubility – solubility product – common ion effect – precipitation methods – co –precipitation – condition of precipitation – preparation from homogeneous solutions – purity of precipitates

General discussions of complexometric titrations, stability constants – Different ways of expressing stability of complexes, EDTA titrations – different types, masking and demasking agents, Metal ion indicators – Eriochrome Black – T, xylenol orange and murexide – Determination of hardness of water using EDTA – Determination of the following metal ions using EDTA – Zn, Mg, Ca, Mn and Ni

### **Unit III : Chromatography**

Column chromatography – Adsorption and partition – Simple elution – Stepwise or fractional elution – Gradient elution analysis – Adsorbents – Solid supports, Frontal analysis, Displacement development analysis, Ion exchange chromatography – Principle, classification and application – Elutropic series – selectivity of resins, gel chromatography, gas chromatography, gas – solid and gas – liquid – theory, technique, details of various components of apparatus – carrier gas – column – detectors – recorders – applications – molecular sieves – high performance liquid chromatography – electrophoresis & HPTLC – moisture determination – Karl Fischer titration.

### **Unit IV : Electroanalysis**

Direct potentiometry – Null point potentiometry, potentiometric titrations – Conductometric titrations - Coulometry and amperometric titrations – principle and instrumentation, primary and secondary coulometric analysis, coulometry at controlled potential – Coulometry at constant current – Separation of nickel and cobalt by coulometry

### **Unit V : Diffraction methods for structural studies**

Crystal Structure - 7 Crystal Systems - 14 Bravais Lattices - Cubic Crystals Characterization of Structure - X – ray diffraction – A brief account of the principles of molecular structure determination by X-ray diffraction from single crystal – structure factor, Phase problem and heavy atom methods, Patterson synthesis, Fourier Synthesis, Interpretation of Fourier Maps and results.

Neutron diffraction - Applications of neutron diffraction to studies of molecular structure, advantages over X- ray diffraction studies

Electron diffraction – principles of electron diffraction and applications

**Text Books:**

1. A.I. Vogel, "Textbook of quantitative analysis", 5<sup>th</sup> edition, 1994 by G.H. Jeffery, J. Bassett, J. Mendham & R.C. Donney, ELBS, 1994
2. Douglas A. Skoog, Donald M. West and F. James Holler, "Analytical Chemistry and Introduction", Saunders, College publishing, New York, 1990
3. Douglas A. Skoog and James J. Leary, "Principles of Instrumental Analysis", 4<sup>th</sup> edition, Saunders, College publishing, New York, 1992
4. A.V. Ebsworth, D.W.H. Rankin and S. Cradok, "Structural Methods in Inorganic chemistry", Blackwell publications, ELBS, London, 1988
5. C.N.R. Rao and J. Gopalakrishnan, "New Directions in Solid State Chemistry"; 2<sup>nd</sup> Edition; Cambridge University Press, 1997

**Reference Books:**

1. H.A. Willard and L.L. Merrit, J.A. Dean, "Instrumental methods of Analysis", Van Nostrand, New York, 1986
2. Gary D. Christain and James E. O'Reilly, "Instrumental analysis" 2<sup>nd</sup> edition, Prentice Hall, New Jersey, 1986
3. R.A. Day Jr., A.L. Underwood, "Quantitative Analysis", 6<sup>th</sup> edition, Prentice Hall of India, 1993
4. Silverstein, Francis X. Webster, David Kiemle and David J. Kiemle "Spectrometric Identification of Organic Compounds" John Wiley & Sons Inc., 2003
5. Anthony R. West, "Solid state chemistry and it's applications", John Wiley, 1984

**CH327 PHYSICAL CHEMISTRY - II****Credits:4:0:0****Unit 1 : Chemical kinetics**

Chemical kinetics – over view of first, second and third order reactions – rate law – complex reactions – mechanism – steady state approximation – effect of temperature – Arrhenius treatment – theories of reaction rate – collision – absolute reaction rate – competing and parallel reactions – chain reactions – transition state theory – opposing reactions – consecutive reaction – deduction of rate laws – kinetics of fast reaction – Hammetts relationship – ionic reactions in solution – effect of ionic strength.

**Unit II : Mechanism of gas phase reactions**

Chemiluminescence – reactions in molecular beam – Lindemann's theory – Hinselwood, Kassel and Slater' Streatments – abnormal frequencies – Ortho-para conversions – explosion limits – reaction rates in solution – effect of dielectric constant and ionic strength – kinetic isotope effect – linear free energy relationships – Hammett equation – Taff equation – Yukawa – Tsuno equation – fast reactions – luminescence and energy transformations – study of kinetics of stopped flow techniques – flash photolysis – shock tubes.

**Unit II : Catalysis**

Acid – Base catalysis – general scheme – Arrhenius complex – Vant Hoff's complex – specific and general catalysis – catalytic constants – Bronsted relationship – Hammett acidity functions – mechanism of acid-base catalysed reaction – catalysis by transition metal ions and their complexes, supported transition metal complexes as catalysts – enzyme catalysis – theory and applications

#### **Unit IV : Introduction to quantum mechanics**

The failures of classical physics – heat capacities – black body radiation – The photo electric heat – The Compton effect – The diffraction of electrons – Atomic and molecular spectra, wave particles duality – Uncertainty principle, operators and commutation relations – Postulates of quantum mechanics – Scrodinger equation, Free particle, particle in one dimensional box – Harmonic oscillator – Rigid rotor – Hydrogen atom – Angular momentum – Spin, coupling of angular momentum – Spin-orbit coupling.

#### **Unit V : Quantum chemistry of atoms and molecules**

Variation and perturbation theory – Application to helium atom – Antisymmetry and Pauli's exclusion principle – Aufbau principle – Slater determinantal wave functions – Term symbols and spectroscopic states – Born Oppenheimer approximation – Hydrogen molecule ion – LCAO, MO and VB treatments of hydrogen molecule – Group theory – Character tables – Selection rules – MO treatment of large molecules with symmetry – Hybridization – Huckel theory of conjugated molecules – Cyclic systems – Wood- ward Hoffman rules.

#### **Text Books:**

1. A.W. Adamson, "Physical Chemistry of Surfaces", 5<sup>th</sup> edition, Wiley, 1990
2. K.J. Laidler, "Chemical Kinetics", Harper and Row, New York, 3<sup>rd</sup> Edition, 1990
3. Donald A McQuarrie, "Quantum Chemistry", University Science Books, Mill Valley, California, 1983.
4. AK Chandra, "Introduction to Quantum Chemistry", Tata McGraw Hill, New Delhi
5. John C. Schug, "Introductory Quantum Chemistry", Holt, R & W Publisher, 1972

#### **Reference Books:**

1. J. Rajaram and J.C. Kuriakose, "Kinetics and mechanism of chemical transformation", McMillan India Ltd., New Delhi, 1993
2. C. Kalidas, "Chemical Kinetic Methods: Principles of Relaxations Techniques and application", New Age International (P) Ltd, Chennai, 1996
3. P.W. Atkins, "Molecular Quantum Mechanics", 2<sup>nd</sup> edition, Oxford University Press, 1983
4. I.N. Levine, "Quantum Chemistry", 4<sup>th</sup> edition, Prentice Hall India, 1994
5. M.W. Hanna, "Quantum Mechanics in Chemistry", 3<sup>rd</sup> edition, Addition Wisley, London, 1981

### **CH328 ORGANIC CHEMISTRY - II**

**Credits:4:0:0**

#### **Unit I : Principles of organic synthesis**

The synthesis process – preliminary planning, molecular characteristics, functional group transformation – retrosynthetic analysis – order of events – one group – C – X disconnection – Chemo selectivity two group C- X disconnection – chemo selectivity two group C-X disconnection – reversal of polarity – cyclisation reactions – protecting groups – one group disconnection C-C, alcohols, C+O, stereoselectivity – regioselectivity

## Unit II : Organic name reactions and reagents used in organic synthesis

Organic name reactions: Baeyer – villiger reaction - Hofmann reaction - Favorskii reaction - Michael addition - Mannich reaction - Stork - Enamine reaction - Sharpless asymmetric epoxidation - Ene reaction - Barton reaction - Holmann-Loffer-Freytag reaction - Shapiro reaction - Chichibabin reaction - Skraup synthesis - Fischer – indole synthesis

Use of the following reagents in organic synthesis and functional group transformations - Complex metal hybrids - Gilman's reagent - lithium dimethylcuprate - lithium diisopropylamide (LDA) dicyclohexylcarbodiimide - 1,3 – Dithiane (reactivity umpolung) - trimethylsilyl iodide - tri-n-butyltin hydride - Woodward and provost hydroxylation - osmium tetroxide – DDQ - selenium dioxide - phase transfer catalysts - crown ethers and Merrified resin - Peterson's synthesis - Wilkinson's catalyst - Baker yeast

## Unit III : Pericyclic reaction

Definition – types – FMO treatment, PMO method and correlation approaches and diagrams of typical electrocyclic reactions, cycloadditions, sigmatropic reactions – cope and claisen rearrangement

## Unit IV : Organic Photo Chemistry

Introduction – Interaction of electromagnetic radiation with matter – electronic excitations – excited states – transfer of excitation energy – sensitization and quenching – photochemical eliminations, Norrish type I and II reactions, Paterno-Buchi reaction, oxidations – reductions, cis-trans isomerisation, rearrangements (di-pi methane or Zimmerman rearrangement).

## Unit V : Hetero cyclics and supramolecules

Heterocyclics – Nomenclature – compounds containing two hetero atoms – azoles – chemistry of pyrazole, imidazole, oxazole, isoxazole, thiazole and isothiazole – diazines – pyrimidines.

Supra molecular chemistry – preparation and structure of catenanes and rotaxanes – molecular recognition – synthetic applications of calixarenes and cyclodextrines – organic reactions on solid supports zeolite, clay, alumina and silica.

### Text Books:

1. I.L. Finar, "Organic Chemistry" Vol.2, ELBS, 6<sup>th</sup> edition, Singapore, 1984
2. Robert E. Ireland, "Organic synthesis", 2<sup>nd</sup> edition, Prentice-Hall of India Pvt. Ltd., New Delhi, 1988
3. V.K. Ahluwalia and Ram Aggarwal, "Organic Synthesis", Narosa Publishing House, New Delhi
4. G.R. Chatwal, "Organic photo chemistry" 1<sup>st</sup> edition, Himalaya Publishing House, Mumbai, 1988
5. A. Hassner and C. Stumber, "Organic Syntheses based on name reactions", Pergamon, 2002

### Reference Books:

1. R.O.C. Norman, "Principles of organic synthesis" 2<sup>nd</sup> edition, Chapman and Hall, London, New York, 1978
2. J.M. Coxon, B. Halton, "Organic photochemistry", Cambridge University Press, 2<sup>nd</sup> edition, 1987
3. R.K. Bansal, "Heterocyclic Chemistry", Wiley Eastern, 1990

4. Andre Loupy, "Solvent free reactions", Topics in current chemistry, Vol. 206, Page 155 –173
5. G. Schill. Catenanes, Rotaxanes, and Knots, Academic Press, New York (1971)
6. W. Carruthers, "Some modern methods of organic synthesis", Cambridge university press, 3<sup>rd</sup> edition, 1988
7. T.L. Gilchrist & R.C. Storr, "Organic reaction orbital symmetry", Cambridge university press, 1972
8. F.A. Cavey and R.J. Sundberg, "Advanced Organic Chemistry Part – B: Reactions and Synthesis, Plenum Press, 3<sup>rd</sup> edition, 1990

## **CH329 INORGANIC CHEMISTRY - II**

**Credits:4:0:0**

### **Unit I : Coordination Chemistry**

Introduction - Formation of complexes - Bonding theories for coordination complexes - Crystal Field Theory, Ligand Field Theory, Molecular Orbital Theory, Werner's theory – Stability constant: Experimental determination of stability constant – factors influencing – Stabilization of unusual oxidation states by complex formation – the nature of the metal – ligand bond, molecular orbital theory of a complex and its limitation – Crystal field theory – concept, influence of ligand on CF splitting and limitation – Ligand field theory – Jahn – Teller effect – electronic spectra and magnetic moments.

### **Unit II : Inorganic reaction mechanisms**

Reactions of square – planar complexes – Mechanism of ligand displacement reaction – Substitution in the square planar complexes - mechanism, entering group effect, cis effect and trans effect. Substitution in octahedral complexes – Dissociate and associative mechanisms – Base hydrolysis - Isomerisation reactions – Substitution without breaking the metal –ligand, electron transfer reaction – Outer sphere and inner sphere reactions.

### **Unit III : Organo metallics**

Definition – Types of bonds – Complexes of olefin, acetylene and cyclopentadiene and benzene derivatives – Metallocenes – Fluxional molecules – Homogeneous catalysis – Hydrogenation, carbonyl ion

### **Unit IV : Bio-inorganic chemistry**

Essential and trace metals in biological systems – Metalloporphyrins – Chlorophyll, hemoglobin, myoglobin, vitamin B<sub>12</sub> – iron sulphur proteins – Nitrogen cycle, nitrogen fixation and dinitrogen complexes – anticancer drugs (mainly Pt complexes) and their probable mechanism of action. Metal centered enzymes – structure and function

### **Unit V : Chemistry of cluster compounds and Inorganic polymers**

Preparation, structure and bonding of boron hydrides, carboranes and heteroboranes – properties structure and uses of inorganic polymers of boron, silicon, germanium and tin

#### **Text Books:**

1. B.R. Puri and L.R. Sharma, "Principles of Inorganic Chemistry", Shoban Lal Nagin Chand and Co., 1989

2. D. Banerjee, "Coordination Chemistry", 5<sup>th</sup> edition, ELBS with Chapman and Hall, London, 1996
3. K.K. Rohitgi Mukerjee, "Fundamentals of photochemistry" Wiley Eastern Limited, New Delhi, 1992
4. Madan, Malik, Tuli, Inorganic Chemistry, S. Chand & Company, New Delhi, 2002

**Reference Books:**

1. R.J.P. Williams & J.R.R.F. de Silva, "New Trends in Bio-inorganic Chemistry", Academic Press, London, 1975
2. Ronald D. Archer, "Inorganic and Organometallic Polymers", Wiley-VCH, 2001
3. Florian P Pruchnik, V Pruchnik, "Organometallic Chemistry of the Transition Elements", Springer, 1990
4. William L. Jolly, "Modern Inorganic Chemistry" 2<sup>nd</sup> Edition, McGraw-Hill, Inc., 1991

**CH330 ORGANIC CHEMISTRY LAB**

**Credits:0:0:4**

12 experiments will be notified by the HOD from time to time

**CH331 SOLID STATE CHEMISTRY**

**Credits:4:0:0**

**Unit I. Crystal Chemistry**

Structures of complex oxides and related compounds – defects in solids – origin and types of defects, non-stoichiometry – defects and physical properties – ionic conductivity and optical properties

**Unit II. Preparative methods**

Polycrystalline materials by solid state, preparation, precursor, ion exchange, sol-gel, intercalation methods – high pressure synthesis, preparation of single crystals – different methods – basics of nano technology – preparation of nano materials - preparation of thin films, amorphous and nano crystalline materials.

**Unit III. Characterization of solids**

X-ray diffraction, electron and neutron diffraction – thermal methods – TGA, DTA, DSC and TMA – XPS, Auger, ISS, SIMS, principles and techniques.

**Unit IV. Electrical properties**

Band theory of solids – metals, non-metals, semi conductors – thermopower – hall effect – insulators – measurement of 2 probe and 4 probe methods – dielectric, ferroelectric, pyroelectric and piezoelectric materials – super conductivity – theory – high TC materials.

**Unit V. Magnetic properties**

Dia, para, ferro and antiferromagnetic properties – measurement of magnetic susceptibilities – Guoy and Faraday methods – magnetized solids – soft and hard materials.

**Text Books:**

1. A.R. West, "Solid state chemistry and its applications", John Wiley, 1984
2. C.N.R. Rao and J. Gopalakrishnan, "New Directions in Solid State Chemistry"; 2<sup>nd</sup> Edition, Cambridge University Press, 1997
3. DK Chakrabarty, Solid State Chemistry, New Age Publishers, 1996
4. C. Daniel Yesudian and D.G. Harris Samuel, Materials Science & Metallurgy, Scitech Publishers, 2004

**Reference Books:**

1. Lesley Smart and Elaine Moore, "Solid state chemistry – an introduction", Chapman and Hall, 1992
2. L.V. Azaroff, "Introduction to Solids", Tata McGrawHill, 1990

**CH332 ANALYTICAL CHEMISTRY - II**

**Credits:4:0:0**

**Unit I : Atomic Spectroscopy**

Atomic absorption spectroscopy – principle – instrumentation, single and double beam atomic absorption spectrometer, detection limits and sensitivity – applications - Atomic emission spectroscopy – Types of emission spectra – excitation energy requirement – instrumentation – spectrographs – applications - Atomic fluorescence spectroscopy.

**Unit II: UV – Visible Spectroscopy & Surface morphological determination**

The electromagnetic spectrum – fundamental laws of photometry – deviation from Beer's law – presentation of spectra – correlation of electronic absorption spectra with molecular structure – molar absorptivity – structural effects – effect of temperature and solvents – quantitative methods – UV – visible spectroscopy for structural elucidations - photometric titrations – electron spectroscopy for chemical analysis (ESCA) – Scanning Electron Microscope – Tunneling Electron Microscope

**Unit III : IR - spectroscopy and Raman Spectroscopy**

Selection rules for IR absorption, fundamental, overtone and hot bands – Normal modes of vibration of molecules such as carbon dioxide and water – Factors influencing the number and energy of absorption bands – Characteristic group vibrations – Factors causing shifts in group vibrations – Skeletal vibrations – Finger printing – Double beam IR spectrophotometer – Components and functions – sample handling – Nujol mull and potassium bromide pellet technique - Applications of IR spectroscopy in structural elucidation of molecules.

Raman spectroscopy – Vibrational mode – group frequencies of organic, inorganic and organometallic compounds, factors affecting the group frequencies, study of hydrogen bonding effects, vibrational spectra of ionic, coordination and metal carbonyl compounds.

**Unit IV : Nuclear Magnetic Resonance, Electronic Spin Resonance Spectroscopy & Photoelectron spectroscopy**

Basic definitions of magnetic moment and spin quantum numbers – The chemical shift – Factors affecting the magnitude of chemical shift – The TMS scale, tau and delta values – Spin – spin splitting of AB, A<sub>2</sub>B<sub>2</sub> and ABX systems – Some examples of spin – spin splitting, NMR of typical organic compounds – Ethanol, ethane, limonene, etc. – Internal rotation and NMR – Deuterium exchange reaction – NMR of nuclei other than hydrogen –

mainly  $^{13}\text{C}$  and applications – F.T. NMR and its advantages over conventional NMR – NMR spectroscopy for structural elucidations - Nuclear quadrupole resonance or NQR - X-ray photoelectron spectroscopy (XPS)

EPR – Principles, factors affecting the intensity, position and multiplet structure of the spectra – Hyperfine splitting of some simple systems, zero field splitting – Kramers degeneracy – Applications

### **Unit V : Mass Spectrometry & Thermogravimetry**

Mass spectroscopy – Basic principles – Instrumentation – The mass spectrometer – Isotope abundances – Molecular ion – Metastable ions – Fragmentation processes – Fragmentation associated with functional groups – Alkanes, alkenes, aromatic hydrocarbons, alcohols, aldehydes, carboxylic acids and esters – McLafferty rearrangement and applications – Thermogravimetry (TG) – Derivative thermogravimetry (DTG) – Differential thermal analysis (DTA) – Differential Scanning Calorimetry (DSC) – Instrumentation and applications

#### **Text Books:**

1. C.N. Banwell, “Fundamentals of Molecular spectroscopy”, 3<sup>rd</sup> Edn., Mc-Graw – Hill, New Delhi, 1983
2. J. Dyer, “Absorption Spectroscopy of Organic Molecules”, Prentice Hall of India, 3<sup>rd</sup> Edn., Macmillan, 1991
3. W. Kemp, “Organic Spectroscopy”, 3<sup>rd</sup> Edn., ELBS, 1991,
4. G. R. Chatwal and S.K. Anand, “Instrumental method of chemical analysis”, 5<sup>th</sup> Edition, Himalaya Publishing House, Mumbai 2002

#### **Reference Books:**

1. J.K. Saunders and B.K. Hunter, “Modern NMR Spectroscopy”, Oxford University Press, Oxford, 1987
2. D.H. Williams and I. Fleming, “Spectroscopic methods in Organic Chemistry”, 4<sup>th</sup> edition, Tata McGraw Hill, New Delhi, 1988
3. R.M. Silverstein, G.C. Bassler, T.C. Morrill, “Spectrometric Identification of Organic Compounds”, John Wiley, New York, 1991
4. H.A. Willard and L.L. Merritt, J.A. Dean, “Instrumental methods of Analysis”, Van Nostrand, New York, 1986

## **CH333 PHYSICAL CHEMISTRY - III**

**Credits:4:0:0**

### **Unit I. Group Theory**

Molecular symmetry – symmetry elements and symmetry operations-successive operations, inverse operations - Cartesian coordinate system - relations among symmetry elements - Properties of a group – Abelian, non abelian and cyclic groups - Multiplication tables – classes, subgroups - Molecular point groups - Schoenflies symbols - Matrices of symmetry operations - Representations of a group-Reducible and irreducible, representations - Statement and proof of Great orthogonality theorem - Characters and construction of character table ( $C_{2v}$ ,  $C_{3v}$ ,  $C_{2h}$ ) – Explanation of a character table - Direct product groups

## Unit II. Applications of Group Theory

Standard reduction formula relating reducible and irreducible representations - Symmetries of normal modes of vibration in non-linear molecules ( $\text{H}_2\text{O}$ ,  $\text{NH}_3$ ,  $\text{BF}_3$ ) and in linear molecules ( $\text{C}_2\text{H}_2$ ) - Normal mode analysis - Selection rules for vibrational spectra – IR and Raman active fundamentals – Mutual exclusion rule - Symmetries of M.O and symmetry selection rule for electronic transition in ethylene and formaldehyde - Hybridisation schemes for atoms in ethylene and butadiene – Group theoretical method of obtaining delocalisation energies.

## Unit III. Photo Chemistry

Physical properties of electronically excited molecules – Dipole moment, pKa and redox potentials - Fluorescence, phosphorescence and delayed emission - Stern Volmer equation-Derivation, limitations and applications - Photosensitisation and chemiluminescence - Experimental techniques-Chemical actionometry – Conventional photolysis and flash photolysis - Some photochemical reactions like  $\text{H}_2$  – halogen, decomposition of carbonyl compounds - Elementary ideas of photosynthesis and solar energy conversion.

## Unit IV. Applied Electrochemistry

Theories of electrical double layer (EDL) – EDL at the electrode – electrolyte interface-Helmholtz model of DL - Electrode kinetics – Butler Volmer equation–Derivation of the equations-Tafel equation and plots - Hydrogen overpotential – Mechanism of hydrogen evolution reactions – Theories of hydrogen overvoltage - Passivity (electrical, chemical and mechanical passivity) - Corrosion (definition, theory, methods of preventing corrosion) - Polarography – Dropping mercury electrode – half wave potential and applications – Introduction to Electrochemical energy conversions

## Unit V. Nano Technology

Nanomaterials – Preparation: Plasma arcing - Chemical vapour deposition – Sol-gels – silica gels – Hydrolysis – Condensation and polymerization of monomers to form particles – Zirconia and yttrium gels – Aluminosilicate gels – Forming nanostructured surfaces using the sol – gel process – Trapping by sol –gels – Electrodeposition – Ball milling – Using natural nanoparticles – Applications of nano materials – Insulations materials - Machine tools – Phosphors – Batteries – High power magnets – Motor vehicles and aircraft – Medical applications

### Text Books:

1. K. Veera Reddy, “Symmetry and spectroscopy of molecules”, New Age International (P) Ltd., 2000
2. P.K. Bhattacharya, “Group Theory and its Chemical application”, Himalaya Publishing House, New Delhi, 1986
3. K.K. Rohatgi Mukherjee, “Fundamentals of photochemistry”, Wiley Eastern, New Delhi, 1986
4. Michael Wilson, Kamali Kannangara, Geoff Smith, Michelle Simmons and Burkhard Raguse, “Nanotechnology – Basic Science and Emergin Technologies”, Chapman & Hall (CRC), 2004
5. Samuel Glasstone, “An Introduction To Electrochemistry”, Maurice Press, 2007

### Reference Books:

1. F.A.Cotton, "Chemical application of group theory", 2<sup>nd</sup> edition, Wiley-Interscience, New York, NY, 1971
2. K.V. Raman, "Group theory and its applications to chemistry", Tata Mcgraw Hill, 2004
3. Alan Cox and T.J. Kemp, "Introductory photochemistry", McGraw-Hill, 1971
4. John O'M. Bockris, Amulya K. N. Reddy, "Modern Electrochemistry Vol. I and II", Plenum Publishing, 1970
5. Richard C. Alkire, Dieter M. Kolb, Jacek Lipkowski and Phil Ross, "Advances in Electrochemical Science and Engineering, Volume 9", Wiley, 2006

### CH334 ORGANIC CHEMISTRY - III

**Credits:4:0:0**

#### **Unit – I: Molecular rearrangements**

Mechanism of the following rearrangement reactions – Pinacol-Pinacolone rearrangement – Wagner-Meerwein rearrangement– Hofmann rearrangement– Beckmann rearrangement – Curtius rearrangement – Wolff rearrangement – Baeyer-Villiger reaction – Dakin reaction – Stevens rearrangement – Sommelet rearrangement – Wittig rearrangement – Benzidine rearrangement – Hauser rearrangement – Favorski rearrangement – Benzil-Benzilic acid rearrangement – Cope rearrangement – Dienone rearrangement

#### **Unit – II: Chemistry of Alkaloids and Terpenoids**

General methods of structure elucidation of alkaloids – structure, synthesis and stereochemistry of the following alkaloids – Quinine, Tropine, Cinchonine, Morphine, Papaverine, Lysergic acid, cocaine and reserpine – Biosynthesis of alkaloids  
Terpenoids - Classification - Structure, Stereochemistry and synthesis of alpha – Pinene, camphor, Zingiberene, cadinene, abietic acid and squalene. – Biogenesis of terpenoid

#### **Unit – III: Natural Products– I**

Vitamins - Structural elucidation and synthesis of vitamins A, B<sub>6</sub>, C, D and E - Antibiotics and antibacterials - Antibiotic  $\beta$ -Lactam type - Penicillins - Antitubercular - Streptomycin - Broad spectrum antibiotics - Tetracyclines - Anticancer - Dactinomycin (Actinomycin D) - Antibacterial – Ciprofloxacin, Norfloxacin - Antiviral – Acyclovir - Antimalarials : Chemotherapy of malaria - Antihistaminic and antiasthmatic agents : Terfenadine, Cinnarizine, Salbutamol .

#### **Unit – IV: Natural Products – II**

Steroids – Introduction, Constitutional study of cholesterol, stereochemistry of steroids. Steroid hormones – Structural elucidation of progesterone, androsterone.

#### **Unit – V: Anthocyanidins and Pigments**

Introduction – structure of anthocyanidins – general methods of synthesizing anthocyanidins – Flavones – Iso flavones – Biosynthesis of flavones – Tannins.

#### **Text Books:**

1. I.L.Finar, Organic Chemistry, Vol.2 – ELBS 5<sup>th</sup> Edition, 1989.

- O. P. Agarwal, Chemistry of natural products, Vol.1, Goel publishing house, 15<sup>th</sup> edition, 1992.
- Jerry March, "Advanced Organic Chemistry – Reactions, Mechanisms and structure, 4<sup>th</sup> edition, John Wiley & Sons, 1992
- Gurdeep R. Chatwal, "Reaction Mechanism and Reagents in Organic Chemistry", Himalaya Publishing House, New Delhi
- A. Kar, "Medicinal Chemistry", Wiley Eastern Ltd., New Delhi, 1993
- W. O. Foye, "Principles of Medicinal Chemistry", 3<sup>rd</sup> Edition, Lea & Febiger/Varghese Publishing House, Bombay, 1989

#### Reference Books:

- Francis A. Carey, "Organic Chemistry", 5th edition, Tata McGraw Hill, New Delhi, 2003.
- Graham Solomons T.W, "Organic Chemistry", Vol.I & II, 5th Edn, John Wiley & Sons, New York, 1992.
- O.P. Agarwal, "Organic Chemistry Reactions and Reagents".
- Morrison and Boyd, "Organic Chemistry", 3<sup>rd</sup> edition, United states of America, 1980

### CH335 INORGANIC CHEMISTRY - III

**Credits:4:0:0**

#### Unit I: Metallurgy

Isolation, Purification, properties and uses of Beryllium, Germanium, Titanium, Zirconium, Thorium, Vanadium, Plutonium, Uranium and Platinum. – Preparation and uses of the following compounds: Beryllium - Basic Beryllium acetate, BeCl<sub>2</sub>, Titanium - TiCl<sub>4</sub>, TiO<sub>2</sub>, Zirconium - ZrCl<sub>4</sub>, ZrO<sub>2</sub> (Zirconia), Vanadium - V<sub>2</sub>O<sub>5</sub>, VCl<sub>4</sub>, Uranium - UF<sub>4</sub>, UO<sub>2</sub> (NO<sub>3</sub>)<sub>2</sub> 9H<sub>2</sub>O (Uranyl nitrate), Thorium - ThO<sub>2</sub> (Thoria), Th(NO<sub>3</sub>)<sub>2</sub>, Platinum - PtCl<sub>4</sub> (Platinic Chloride), H<sub>2</sub>PtCl<sub>6</sub> (Chloroplatinic acid)

#### Unit II: Inorganic Polymers

Classification, Types of Inorganic Polymerization - Comparison with organic polymers - Boron-oxygen and boron-nitrogen polymers – silicones - coordination polymers - sulfur-nitrogen -sulfur-nitrogen-fluorine compounds - chalcogenide clusters – binary and multi-component systems - homolytic inorganic systems

#### Unit III: Nonaqueous Solvents

General properties and classification of solvents – Self-ionization and leveling effect – Reactions in nonaqueous solvents – Solute-solvent interaction - Reactions in liquid NH<sub>3</sub> – Solutions of metals in liquid ammonia – Reactions in anhydrous sulphuric acid, liquid SO<sub>2</sub>, liquid HF, liquid halogens and interhalogens, and liquid dinitrogen tetroxide – Titrations in nonaqueous solvents – Acid-base and redox titrations.

#### Unit IV: Molecular Magnetic Materials

Basic concepts of molecular magnetism - Types of magnetic interactions -Recent techniques of magnetic susceptibility measurements - Inorganic and organic ferro-magnetic materials - Low-spin – high-spin transitions - Isotropic interactions in dinuclear compounds (dipolar, anisotropic and anti-symmetric interactions) - Trinuclear compounds and compounds of high

nuclearity - Magnetic chain compounds - Magnetic long-range ordering in molecular compounds: design of molecular magnets, physical investigations and applications

### **Unit V: Inorganic Photo chemistry**

Excited states of Coordination complexes - Properties of excited states, Photochemical pathways - Energy transfer, Charge transfer photo chemistry, Photo redox reactions, Photo substitution reactions - Ruthenium poly pyridines, Chromium polypyridyls, Photochemical conversion and storage of solar energy, Inorganic photo chemistry at semiconductor electrodes

#### **Text books:**

1. F. A. Cotton and G. Wilkinson , “Advanced Inorganic Chemistry”, 6<sup>th</sup> Edn. John-Wiley & Sons, New York, 1999
2. James E. Huheey, “Inorganic Chemistry”, 4<sup>th</sup> Edn., Addison Wesley Pub. Co., New York, 1993
3. Gary L. Miessler and Donald A. Tarr, “Inorganic Chemistry”, 2<sup>nd</sup> Edn., Prentice Hall International Inc., London.,1999
5. Oliver Kahn, Molecular Magnetism, VCH, Weinheim, 1993
6. Harry Sisler, “Chemistry of nonaqueous solvent”, Reinhold, 1961

#### **Reference books:**

1. J. E. Huheey, “Inorganic Chemistry”, 3<sup>rd</sup> Edition, Harper and Row publishers, 1983
2. Harper and Row – Principles of structure and reactivity; International edition, 1972
3. J. Kucharsky and L. Safarik, “Titrations in Nonaqueous Solvents”, Elsevier, 1965
4. Emelius and Sharpe, “Modern Aspects of Inorganic Chemistry”, 4<sup>th</sup> Edition, Wiley, 1973
5. Gurdeep Raj, “Advanced Inorganic Chemistry”, Goel Publishing House, 2002
6. Catherine Housecroft and Alan G. Sharpe “Inorganic Chemistry”, Prentice Hall, 2007

### **CH336 PHYSICAL CHEMISTRY LAB**

**Credits:0:0:4**

12 experiments will be notified by the HOD from time to time

### **CH337 ENVIRONMENTAL CHEMISTRY**

**Credits:4:0:0**

#### **Unit I. Environment**

Introduction – components of environment – factors affecting environment – types of environment – environmental management – objectives and components of environmental management.

Environmental education – objectives – principles environmental education – environmental educational programmes – health and environment – women and environment – environmental protection act – concept of environmental chemistry – segments of environment – environmental pollution – introduction – origin of pollution – pollutant – classification of pollutants – types of pollution

#### **Unit II. Chemistry of the pollution of the atmosphere**

Introduction – Composition of Air-sources of air pollution – particulate matter – automobile emission – gaseous pollutants – sources and effects of the oxides of nitrogen, sulphur and carbon – Control of CO<sub>x</sub>, NO<sub>x</sub>, SO<sub>x</sub>, hydro carbons and particulates.

Gaseous and sedimentary cycles – nitrogen cycle, oxygen cycle, carbon cycle, photolytic cycle of NO<sub>2</sub>, sulphur cycle and phosphorous cycles, green house effect – natural sources of green house effects – global warming

Ozone layer – formation of ozone – mechanism of ozone depletion – effects of ozone depletion – ozone hole - Acid rain – introduction – effects acid rain – control – Analysis of CO, NO<sub>x</sub>, SO<sub>x</sub> and hydrocarbons

### **Unit III. Chemistry of the pollution of hydrosphere**

Introduction –classification of water pollution – physical pollution – chemical pollution – biological pollution and physiological pollution.

Ground water, surface water, lake water, river water, sea water pollution – sources and effects – Classification of water pollutants – inorganic pollutants and toxic metals – detrimental effects of inorganic pollutants – organic pollutants – effects of organic pollutants – oxygen demanding waste – disease causing agents, land nutrients, sediments, oil.

Eutrophication – introduction – types of eutrophication effects and control of eutrophication

Thermal pollution – sources and effects – control of thermal pollution – water control of thermal power plant – prevention of thermal pollution – measurement of thermal pollution.

### **Unit IV. Water treatment and sewage treatment**

Water treatment – introduction – softening of water – clark's process – lime soda process – ion exchange process – demineralization of water – determination of hardness – treatment of water for municipal purpose – chemical methods of sterilization - physical method of sterilization – terms of chlorination – electro dialysis method – reverse osmosis method – coagulation of water – flocculators.

Sewage treatment – municipal waste water – sewage and its composition – methods of sewage treatment – preliminary or mechanical treatment, primary treatment – secondary treatment – activated sludge process – sludge disposal – need for sludge disposal – tertiary treatment.

### **Unit V. Chemistry of pollution of lithosphere**

Soil pollution – sources – Industrial waste, urban waste, radioactive waste, agricultural practices, chemical and metallic pollutants, biological agents – detrimental effects of soil pollutants – effects of industrial pollutants and urban waste.

Pesticides – types – environmental effects of pesticide pollution – control pollution of radioactive waste – sources and effects somatic and genetic effects – transmission of radiation to man control

Solid waste – types and sources – effects of solid waste – solid waste collection – disposal in sanitary land fills, incineration, pyrolysis and composting – recycling solid waste.

#### **Text Books:**

1. S.M. Khopkar, "Environment Pollution Analysis", New Age International (P) Ltd. Publishers, New Delhi, 1993

2. B.K. Sharma & H. Kaur, "Environmental Chemistry", Goel Publishing House, Meerut, 1994
3. S.S. Dara, "A Textbook of Environmental Chemistry and Pollution Control", S. Chand & Company Limited, New Delhi, 1995

**Reference Books:**

1. JO'M Bockris (ed), "Environmental Chemistry", Plenum Press, New York, 1977
2. John W Moore and Elizabeth A Moore, "Environmental Chemistry", Academic Press, New York, 1976
3. Colid Baird, "Environmental Chemistry" WH. Freeman and Company, New York, 1995

## **CH338 PETROLEUM CHEMISTRY**

**Credits:4:0:0**

### **Unit I. Theories of petroleum and refining**

Introduction – theories of origin of petroleum – Refining, Distillation – theory – McCabe – Thiele plate method, fractional distillation, separation, operations involved in refining – constituents of petroleum

### **Unit II. Cracking and refining**

Thermal, catalytic and hydro cracking – mechanisms of catalytic cracking for primary and secondary reactions – Reforming reactions – Alkylation – Mechanism of catalytic alkylation – isomerisation, polymerization, hydrodesulphurisation – finishing process – removal of water, sulphur and particulate impurities – solvent refining.

### **Unit III. Properties and Characteristics of fuels**

Fuel oils – Gasoline – Diesel oils – properties and specifications of a good fuel – knocking – octane and cetane numbers – improvement of anti-knock characteristics of fuel – test methods for petroleum product – specific gravity, flash point, aniline point, calorific value, sulphur, ash content and carbon residue.

### **Unit IV. Lubricants and synthetic petrol**

Lubricants – types – lubricating oil – manufacture – its mechanism of action – semisolid lubricants – properties – detergents – synthetic lubricants

LPG, heating oil, asphalt, synthetic petrol – methods of production – Fischer – Tropsch method, Bergius process mechanisms.

### **Unit V. Petrochemicals**

Petro chemicals – manufacture of various aliphatic compounds – ethylene production by thermal cracking – mechanisms of propane and naphtha cracking – acetylene processes – manufacture of aromatic hydrocarbons – production of NH<sub>3</sub> and Urea.

**Text books:**

1. Gopala Rao and Sittig, "Outline of Chemical Technology", Affiliated to East West press Pvt. Ltd., New Delhi, 2<sup>nd</sup> edition, 1973

2. R.N. Seireve and J.A. Brink, "Chemical process industries", McGraw Hill International Book Co., London, 4<sup>th</sup> edition, 1977
3. Peter Wireman, "An Introduction to Industrial Organic Chemistry", Applied Sciences publishers, London, 2<sup>nd</sup> edition, 1979

**Reference books:**

1. W. Francis, "Fuels and Fuel Technology", Pergamon Press, London, 1965
2. L.A. Munro, "Chemistry in Engineering", Prentice Hall Inc., London, 1964

**CH339 ADVANCED PHARMACEUTICAL CHEMISTRY**

**Credits:4:0:0**

**Unit I. Introduction to drug design**

Introduction to drug design, physical and chemical factors associated with biological activities, mechanism of drug action, drug dosage, drug delivery systems, drug manufacture – classification of drugs based on structure or pharmacological basis with examples – mechanism of chemotherapeutic action – drug absorption across biological membrane – metabolism of drugs – formulation of drugs – Quality structure activity relationship

**Unit II. Drug discovery at the enzyme level**

Drug discovery at the enzyme level – chemical models and mimics for enzymes – receptor peptides, carbohydrates and other bioactive molecules – enzyme inhibitors – design and synthesis – DNA – protein – interaction and DNA – drug interaction - enzymes in organic synthesis and combinatorial chemistry

**Unit III. Drug action and drugs**

Drug action – Ideal requirement of a drug – sources of drug plant and animal origin – synthetic and semisynthetic drug – terminology and description of terms – Pharmacology, pharmacy, molecular pharmacology, pharmacognesy, pharmao kinetics, pharmaco dynamics – metabolites and anti – metabolites – pharmacophore – bacteria, fungi, virus – structure, sources, disease produced – analgesics – narcotic analgesics – morphine, analogues and modifications – codeine – synthetic narcotic antagonists – pethidines and methodones – narcotic analgesics – nalophine – antipyretic analgesics – pyrazole – salicylic acid – para aminophenol derivatives – aspirin and salol – Drug delivery systems - targeted drugs – anticancer drugs

**Unit IV. Synthesis of secondary metabolites from plants**

Synthesis of secondary metabolites from plants – Techniques of selecting cell lines for high yields of secondary compounds with reference to steroids, alkaloids, saponins, pigments and flavanoids – cell cloning, visual or chemical analysis – factors affecting large scale production of useful chemicals – Drug discovery in cancer research – drugs of plant origin – Cyclophosphamide, Decarbazine, 5 – Fluorouracil, Azathioprine – harnessing the power of genome in the search for new antibiotics, conceptual and practical aspects of monoclonal antibody production – production of antibodies in biomedical research – dual discoveries in tropical diseases and cardio-vascular diseases.

**Unit V. Bioprocess**

Drug production by biotechnological processes – Bioprocess – microbial organisms – bacterial and yeast strains – industrial fermentation process – bio reactors types – bio product recovery and purification – bio process and enzyme technology – application of biotechnology in drug production – Basic concepts of cheminformatics.

**Text books:**

1. R.S. Satoskar and S.D. Bhandarkar, “Pharmacology and pharmacotherapeutics” Vol. I and II, S. Chand & co., Revised edition, 1993
2. Bentley and Driver, “Text book of pharmaceutical chemistry”, Oxford University press, London, 1985 (revised by L.M. Artherden)
3. D. Balasubramanian, “Concept of Biotechnology”, University press, 1996
4. G.L. David Krupadanam, D. K. Varaprasada Rao, K.L.N. Reddy and C. Sudhakar, “Drugs”, Universities Press publication, 2001
5. J.H. Noordik, “Cheminformatics Developments: History, Reviews and Current Research”, IOS press, 2004
6. D R Flower, “Drug Design”, Royal Society of Chemistry, 2003
7. Annette Beck-Sickinger and Peter Weber, “Combinatorial Strategies in Biology and Chemistry”, John Wiley and Sons, 2002

**Reference books:**

1. G.L. Patrick, “Introduction to medicinal chemistry”, Oxford University Press, 1995
2. F.S.K. Barar, “Essentials of Pharmacotherapeutics”, S. chand & Co., 1989
3. G.R. Marshal, “Buyer’s Medicinal Chemistry and Drug Discovery –Principles and practice” M.E Wolff, John Wiley & Sons Inc., New York, 1995
4. V.S. Malik, Padma Sridar, “Industrial Biotechnology” Oxford and IBH publication, 1992
5. “Commercial Biotechnology” – An international analysis, ISBN, Elsevier Science Publication, Pergamon Press, 1984
6. R.K. Murray, D.K. Granner, P.A. Mayes and V.W. Rod well, “Harpers Biochemistry”, 25<sup>th</sup> edition, Appleton and Lange, New York. 2000
7. H.R. Mahler and E. H. Cordes, “Biological Chemistry”, Harper and Row, New York, 1966
8. Dixen and Webb, “Enzymes”, IRL Press, 1979
9. , L. A. Herzenberg, W. M. Weir and C. Blackwell, “Immunochemistry and Molecular Immunology”, Blackwell Scientific Publications, Cambridge, 1996
10. Glazer and Nikaido, “Microbial Biotechnology”, Freeman Press, 1995
11. Bernard R. Glick and Jack J. Pasternak, “Molecular Biotechnology”, 2<sup>nd</sup> edition, American Society for Microbiology, 1998
12. “Science” Vol. 287, March 2000
13. “Protein targets for structure based drugs design” Walkinshaw, Med. Res. Rev., pp.317-372, 1992

**CH340 INDUSTRIAL ELECTROCHEMISTRY**

**Credits: 4:0:0**

**Unit I. Metal Finishing**

Fundamental principles, surface preparation-Electroplating of copper, nickel chromium, zinc and precious metals (gold & silver)- Electroplating for electronic industry- Alloy plating, brass plating- Electroless plating of nickel- anodizing – Electroforming - Electrowinning

### **Unit II. Conducting polymers and Electrochemicals**

Electropolymerisation- anodic and cathodic polymerization-effect of reaction parameters on the course of the reaction- Electrochemical preparation of conducting polymers- Electrolytic production of perchlorates and manganese dioxide- Electro organic chemicals- constant current electrolysis.

### **Unit III. Batteries and Power Sources – I**

Principles of energy conservation- electrochemical energy conservation- thermodynamic reversibility, Gibb's equation. EMF- battery terminology, energy and power density- Properties of anodes, cathodes, electrolytes and separators- Types of anodes, cathodes- Types of electrolytes- Classification of battery- primary and secondary.

### **Unit IV. Batteries and Power Sources – II**

Primary batteries- Dry Leclanche cells, alkaline primary batteries, Zn/air, Lithium batteries- construction, characteristics, problems associated with system- Secondary batteries- Lead acid, nickel cadmium- Fuel cells- Introduction, types of fuel cells, advantages.

### **Unit V. Electrochemical Material Science**

Solar cells- Preparation of CdS/Cu<sub>2</sub>S solar cells by screen printing techniques and their characteristics - Amorphous silicon solar cells - Photo electrochemical cells(PEC) for conversion of light energy to electrical energy - PEC cells based on CdSe and GaAs- characteristics - Introduction to Electrochromism

#### **Text books:**

1. D.Pletcher and F.C.Walsh, "Industrial electrochemistry", Chapman and Hall, London 1990
2. A.T.Khun, "Industrial Electrochemistry", Elsevier Publishers, 1972

#### **Reference books:**

1. N.V.Parthasarathy, "Electroplating and analysis"
2. M.M.Baizer, "Organic electrochemistry", Dekker Inc. New York, 1983
3. M. Barak, "Electrochemical power sources", I.EEE series, Peter Peregrinus Ltd, Steverage, U.K. 1980, reprinted during 1997
4. K.L. Chopra and I. Kaur, "Thin film devices and their application", Plenum Press, New York, 1983
5. Bruno Scrosati, "Applications of Electroactive polymers", Chapman & Hall, London, 1993

## **CH341 BIOCHEMISTRY**

**Credits: 4:0:0**

### **Unit I. Cell and its functions**

Cell structure and functions – chemistry of carbohydrates – structure and properties – biological importance – digestion and absorption of carbohydrates – chemistry of lipids –

biological functions – classification and structure of simple lipids, compound lipids – structure and activities of phospho lipids, glyco lipids, derived lipids, sterols, bile acids.

Transport of materials in the organism – mechanical transport, diffusion transport, active transport, electrophoretic transport, vascular transport –localisation of material transport in the organism – the metabolism of inorganic elements and water

### **Unit II. Chemistry of Biomolecules**

Chemistry of proteins – structure of amino acids, poly peptides and proteins – characterization of proteins – denaturation function – chemistry of nucleic acids – structure and general characterization – compounds of nucleotides and their elucidation – biological importance – structure of DNA and RNA and its functions

### **Unit III. Enzyme and its action**

Enzymes – chemical nature and structure – properties – factors affecting enzyme activity – classification and nomenclature – structural and functional organization of enzymes – co-enzymes – functions – NAD, NADP, flavoproteins, ubiquinones, cytochrome, metal ions as enzyme co-factors – the mechanism of enzyme action – specificity of enzymic action – kinetics of enzymic activity – estimation of enzymic activity – regulation of enzymic activity – multi enzyme complexes

Biological oxidation process by oxygen or loss hydrogen – respiratory chain – oxidation potential - oxidative phosphorylation – mechanism – substrate level phosphorylation – energy rich compounds – Trans phosphoregulation – production of energy in photosynthetic organisms – photosynthesis – mechanism

### **Unit IV. Intermediary metabolism**

Metabolism of carbohydrates – source of glucose – utilization of glucose – storage of carbohydrates – glycogenolysis – glycolysis – EM pathway – Kerb's cycle – Pentose pathway – energetics of glycolysis and glycogenolysis – glucose tolerance – blood sugar level and it's regulation.

Metabolic regulation in various metabolisms – enzymes compartmentation – kinetic factors – chemical modification of regulatory enzymes – cascade system – repression and induction

### **Unit V. Role of Proteins and Nucleic acids and lipid metabolism**

Metabolism of proteins – Digestion and absorption – Oxidative deamination – Transamination – catabolism of some important amino acids – lysine, phenylamine, valine, methionine, cystine – biosynthesis of protein – genetic code – disposal of nitrogen – urea cycle – metabolism of nucleic acids – metabolism of phosphoric acid, pentoses, pureness and hystidines – genes – their repair – mutation – recombination – cloning.

Metabolism of lipids – Digestion and absorption of lipids – Oxidation of fatty acids –  $\beta$  - oxidation pathway – energetics of fatty acids oxidation – oxidation of unsaturated fatty acids – ketosis – ketogenesis – ketolysis – metabolism of phospholipids and glycolipids.

### **Text books:**

1. Lehinger, "Principles of Biochemistry", CBS publishers & distributors, Delhi, 1982
2. G.R. Agarwal and O. P. Agarwal, "Text book of Biochemistry", Goel publishing House, 1984
3. L. Styrer, "Biochemistry", Free man & Co., New York, 1994
4. Michael Yudkin and Robin Offord, "A guide book to Biochemistry", Cambridge University Press, 1971

**Reference books:**

1. R.J. Simond, "Chemistry of Bio-molecules" Royal Society of Chemistry, London, 1992
2. D.E. Metzger, "The Chemical reactions of living cell" Academic press, 1977
3. H. Dugas, "Chemical approach to enzyme action", 2<sup>nd</sup> edition, Springer – Verlay, 1989
4. Abraham White, Philip Hanlec Emil, L.Smith, "Principles of Biochemistry", McGraw Hill, Kogakusha Ltd., Tokyo, 1973
5. E.E. Conn, P.K. Stumpe, "Outlines of Biochemistry", Wiley Eastern Ltd., New Delhi, 1985
6. G. Zubay, "Biochemistry", 2<sup>nd</sup> edition, MacMillan publishing Co., New York, 1988
7. R.K. Murray, P.A., Mayes, D.K. Granner and V.W. Rodwell, "Harper's Biochemistry" (Lange Medical Book), 1990
8. B.L. William and K. Wilson, "Principles and Techniques of practical Biochemistry", Edward Arnold, London, 1995
9. J. Jeyaraman, "Laboratory manual of Biochemistry", Wiley Eastern, 1988

## CH342 POLYMER CHEMISTRY

**Credits:4:0:0**

### Unit I. Basic concepts of polymers

Basic concepts of polymers – classification of polymers – ladder, star comb polymers tacticity – interpenetrating networks – structure property relationships – naturally occurring polymers – polysaccharides – cellulose and proteins – polymerization reactions – classifications – polymer resins – polymer solutions – reaction of polymers – introduction of new groups – cross linking, isomerisation, cyclisation and degradation reactions

### Unit II. Principles of polymerization

Principles of polymerization – step growth polymerization – reactivity of functional groups – carothers equation – kinetics – characteristics of step growth polymerization – examples – mechanisms, choice of monomers, effect of inhibitors or retarders, thermodynamics of free radical, ionic and co-ordination polymerization – examples – co-polymerization – monomer reactivity – ratio – composition, types, the Q-e scheme.

### Unit III. Polymer stereochemistry

Polymer stereochemistry – amorphous, crystalline and crystallites – viscous flow – viscosity, T<sub>g</sub>, T<sub>m</sub> and their relationships – Rheological equations of state – time dependent fluids – elastic effect of polymers – thermal behavior of polymers

#### **Unit IV. Polymerization processes**

Polymerization processes – bulk, solution, emulsion and suspension – industrially important polymers and their polymerization processes – polythene – poly vinyl chloride – poly styrene – phenolic resin – epoxy resin nylon 6,6 – PET – silicone – Teflon – polycarbonate – natural rubber – elastomers or synthetic rubbers – structure – preparation, properties and uses of Buna-S, Buna-N, Neoprene, Thiokol rubbers

#### **Unit V. Conducting Polymers and their applications**

Ion conducting polymer materials - Polymer electrolytes – Solutes for polymer electrolytes – Electro-polymerization of conducting polymer films – Electrochemical impedance of conducting polymers – Highly conductive conventional polymer electrolytes – Plasticizing salts – Lithium batteries with polymer electrodes – Principles of batteries using conductive polymers - Materials used in conductive polymers – Polyacetylene – Polypyrrole – Polyaniline

#### **Text books:**

1. A. Rudin, “The elements of polymer science and engineering”, Academic press, New York, 1982
2. V.R. Gowariker, “Polymer Science”, 5<sup>th</sup> edition, Wiley Eastern Ltd., 1992
3. G.S. Misra, “Introductory polymer chemistry”, New Age International Pvt. Ltd., 1996
4. Anil Kumar and S.K. Gupta, “Fundamentals of polymer science and engineering” Tata McGraw Hill Publication Ltd., New Delhi, 1978
5. Bruno Scrosati, “Applications of Electroactive polymers”, Chapman & Hall, London, 1993

#### **Reference books:**

1. David Sobolev, “A first course in polymer chemistry”, MIR publishers, Moscow, 1971
2. R.J. Young, “Introduction to polymers” Chapman and Hall Ltd., London, 1981
3. D.H. Morton and Jones, “Polymer processing” Chapman and Hall, London, 1989
4. J.A. Brydson, “Plastic materials” 4<sup>th</sup> edition, Butterworth –Heinmann Ltd., London, 1995
5. J.A. Biesenberger and H. Sebastian, “Principles of polymerization engineering” , Wiley Interscience publications, New York, 1988
6. Stephen and Rosen, “Fundamental principles of polymeric materials” 2<sup>nd</sup> edition, John-Wiley and Sons Inc., New York, 1993

### **CH343 INSTRUMENTAL METHODS OF ANALYSIS**

**Credits:4:0:0**

#### **Unit I**

##### **a) Basic Principles in Spectroscopy**

Electromagnetic radiation – Interaction of electromagnetic radiation with matter – absorption, emission, reflection, refraction, dispersion, transmission, polarization and scattering – Uncertainty relation – line width and line broadening – transition probability – transition moment – charge transfer transition – selection rules – intensity of spectral lines – Born Oppenheimer approximation – Fourier transformer – relaxation process

## **b) Atomic absorption and Atomic Emission spectroscopy (AAS / AES)**

Atomic absorption spectroscopy (AAS) – principles – Qualitative analysis – Instrumentation – Detection limits and sensitivity – applications – Flame photometry – Instrumentation – Quantitative analysis – applications

Atomic Emission spectroscopy (AES) – principles of AES – Excitation of energy levels of spectra – types of emission spectra – Instrumentation – quantitative analysis – applications

## **Unit II**

### **a) Ultraviolet and Visible spectroscopy**

Various electronic transitions ( 180 – 800 nm) – Beer – Lambert law – theory of electronic and molecular absorption spectra – effect of solvent on electronic transitions – UV bonds for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polymers – Fieser Woodward rules for conjugated dienes and carbonyl compounds – UV spectra of aromatic compounds – steric effect in biphenyls – UV spectra in quantitative analysis – Instrumentation – visible spectroscopy – basics principles – instrumentation – application in quantitative analysis

### **b) Vibration spectroscopy – Infra red spectroscopy**

Origin of molecular spectra – vibration of poly atomic molecules – selection rules for IR absorption – fundamental, overtones and hot bands – characteristics of groups vibrations – factors influencing shift in group vibrations – skeletal vibration – Finger printing – factors affecting the band positions and intensities – various IR regions – Instrumentation – sample handling – Applications of IR spectroscopy in structural elucidation

Theory of Raman spectroscopy - selections rules – mutual exclusion principle - changes in polarisability – Raman depolarization ratio – factors affecting the group frequencies – Comparison of Raman spectra and IR spectra – interpretation of Raman spectra – Instrumentation – Applications

## **Unit III**

### **a) NMR spectra**

Basic principles of NMR – Chemical shift – spin – spin coupling – shielding mechanism – chemical shift and measurements in NMR – spin – spin coupling or splitting of AB, A<sub>2</sub>B<sub>2</sub> and ABX systems – Examples for the study ; ethanol, propane, benzaldehyde, phenylacetylene and m-cresol – Internal rotation in NMR studies – Deutrium exchange reaction – NMR instrumentation – C<sup>13</sup> NMR – basic principles and applications – FTNMR

### **b) Electron Spin Resonance Spectroscopy**

Basic principles – Zero field splitting and Kramer's degeneracy, factors affecting the 'g' value – Isotopic and anisotropic hyperfine splitting and constants, measurement technique of ESR – instrumentation – applications.

### **c) Molecular Fluorescence Spectroscopy**

Principle – Instrumentation – representation of fluorescence spectra – theory of molecular fluorescence – Relaxation process – Structure and fluorescence – Applications

## **Unit IV**

### **a) Mass spectrometry**

Theory of mass spectrophotometry – Instrumentation – resolution – sensitivity – ionization methods and analyzer molecular ion – odd and even electron ion – fragmentation pattern – rearrangements of ions – meta stable ion and peak – exact masses of nuclides – cleavage of molecules – hydrogen transfer rearrangements – afferty rearrangement and Retro Diels – Alder fragmentation – nitrogen rule – structure elucidation of organic compounds with respect to mass spectral fragmentation pattern – High resolution mass spectrophotometry

### **b) Thermogravimetry**

Principles of thermogravimetry (TG) – Factors influencing thermograms – instrumentation – principles of Derivative thermogravimetry (DTG) – factors influencing thermogram – instrumentation – Principles of Differential thermal analysis (DTA) – instrumentation – examples under study –  $\text{CuSO}_4 \cdot 5 \text{H}_2\text{O}$ ,  $\text{CaC}_2\text{O}_4 \cdot \text{H}_2\text{O}$

### **b) Chromatography**

Basic principles of Chromatography – Gas Chromatography (GC) and Gas – liquid chromatography (GLC) – instrumentation – application – High Pressure liquid Chromatography (HPLC) – application - interpretation

## **Unit V**

### **a) X – ray methods**

x- ray production – basic of crystal structure of materials – X – ray diffraction by crystal lattices – Bragg’s equation – Experimental methods of x-ray diffraction – Lane photograph method, the rotating crystal method, Oscillating crystal method and the powder method – interpretation of the diffraction pattern – Applications

### **b) Electron Spectroscopy (ESCA)**

Principles – Chemical shifts – Instrumentation – x- ray sources – sample analysis – detectors – Recording devices – applications – Auger Electron Spectroscopy (AES) and Ultra violet photoelectron spectroscopy (UPS) – principles – Instrumentation – applications  
Scanning electron microscopy (SEM) and Scanning Tunneling Microscopy (STM) – principles – interpretation of results  
Polarimetry – principles – spectropolarimetry – optical rotatory dispersion – circular dichorism – instrumentation - applications

### **Text books:**

1. A.I. Vogel, “Textbook of quantitative analysis”, 5<sup>th</sup> edition, 1994 by G.H. Jeffery, J. Bassett, J. Mendham & R.C. Donney, ELBS, 1994
2. Douglas A. Skoog, Donald M. West and F. James Holler, “Analytical Chemistry and Introduction”, Saunders, College publishing, New York, 1990
3. Douglas A. Skoog and James J. Leary, “Principles of Instrumental Analysis”, 4<sup>th</sup> editon, Saunders, College publishing, New York, 1992
4. G. R. Chatwal and S.K. Anand, “Instrumental Methods of Chemical Analysis”, 5<sup>th</sup> edition, Himalaya Publishing House, 2002
5. D.A. Skoog, F.J. Holler, T.A. Niemann, “Principles of Instrumental Analysis” (fifth edition) ; Harcourt Brace college ; Philadelphia, PA, 1998
6. R.J. Abraham and P. Loftus, “Proton and carbon  $\text{C}^{13}$  NMR” Heyden, London, 1978

### **Reference books:**

1. H.A. Willard and L.L. Merrit, J.A. Dean, "Instrumental methods of Analysis", Van Nostrand, New York, 1986
2. Gary D. Christain and James E. O'Reilly, "Instrumental analysis" 2<sup>nd</sup> edition, Prentice Hall, New Jersey, 1986
3. R.A.Day Jr., A.L. Underwood, "Quantitative Analysis", 6<sup>th</sup> edition, Prentice Hall of India, 1993

### CH344 NATURAL PRODUCTS CHEMISTRY

**Credits:4:0:0**

#### **Unit – I: Basics of Natural products**

Classification of natural products – classification based on chemical structure, physiological activity, taxonomy and biogenesis - Basics of Bio molecules – Carbohydrates , Amino acids, Nucleic acids – DNA, RNA – Enzymes

#### **Unit – II: Chemistry of natural products**

Structural elucidation and synthesis of the following terpenoids and alkaloids.

Terpenoids – monocyclic sesquiterpenoids – Zingiberene – Bicyclic sesquiterpenoids – Endesmol. Diterpenoids – phytol - Tri terpenoids – squalene.

Alkaloids – Tropaine alkaloids – Atropine – Quinoline alkaloids – Quinine, cinchonine – opaparerine – opium alkaloids – morphine.

#### **Unit – III: Bio-Organic Chemistry – I**

**Vitamins:** Structural elucidation and synthesis of vitamins A, B<sub>6</sub>, C, D and E.

**Drugs:** Structural elucidation and synthesis of penicillins, chloramphenicol and streptomycin.

#### **Unit – IV: Bio-Organic Chemistry – II**

Steroids – Introduction, Constitutional study of cholesterol, stereochemistry of steroids. Steroid hormones – Structural elucidation of progesterone, androsterone.

#### **Unit – V: Anthocyanidins and Pigments**

Introduction – structure of anthocyanidins – general methods of synthesizing anthocyanidins – Flavons – Isoflavones – Biosynthesis of flavones – Tannins.

#### **Text Books:**

1. I. L. Finar, Organic Chemistry, Vol.2, ELBS 5<sup>th</sup> Edition, 1989.
2. O. P. Agarwal, Chemistry of natural products, Vol.1, Goel publishing house, 15<sup>th</sup> edition, 1992
3. A. Berger, "Medicinal Chemistry" Wiley Inter Science, New York (Vol.I and II), 1990
4. O. Wilson, O. Giswold & F. George, "Text book of Organic Medicinal and Pharmaceutical Chemistry", Lippincott Co., Philadelphia, 1991
5. Gareth & Thomas, "Medicinal Chemistry", John Wiley & Son , 2000
6. A. R. Gennaro, "Remington's Pharmaceutical Science", Mac Publishing Co., 1985
7. Arthur C. Guyton, M.D "Text book of Medical Physiology", W.B. Saunders Company, 1996

#### **Reference Books:**

1. Francis A. Carey, "Organic Chemistry", 5<sup>th</sup> edition, Tata McGraw Hill, New Delhi, 2003
2. Graham Solomns T.W, "Organic Chemistry", Vol. I & II, 5th Edn, John Wiley & Sons, New York, 1992
3. Bently and Drivers, "Pharmaceutical Chemistry", Oxford University Press, London, 1985
4. Ashutosh Kar, "Medicinal Chemistry", Wiley Easter Ltd., Chennai, 1992
5. I.L. Finar, "Stereo chemistry and Chemistry of natural products", Volume 2, 5<sup>th</sup> edition, Longman company Ltd., London, 1991

## CH345 CHEMISTRY OF DYES AND PIGMENTS

**Credits: 4:0:0**

### Unit I: Colour

Dye – definition, sensation of colour, colour and constitution - auxochrome, chromophore, Quinonoid theory.

Classification of dyes based on chemical composition, application - acid dyes – basic dyes – direct dyes – mordant dyes – vat dyes – ingrain dyes – food dyes. Important natural dyes.

### Unit II: Direct and Reactive dyes

Direct dyes – Classification, mechanism and application of direct dyes, fastness properties - light, washing fastness

Reactive dyes – Procion (hot, cold brand), Vinyl Sulphone dyes – application on cotton fibers, fastness properties – light, washing fastness

### Unit III: Vat and Azo dyes

Vat dyes – classification – indigoid, anthraquinonoid dyes, application, washing and light fastness.

Azo dyes – principles governing azo coupling –mechanism of diazotiation – coupling with amines, coupling with phenols – classification. – Tautomerism in azo dyes.

### Unit IV Other synthetic dyes

Synthesis, reactions and applications of Di and Triphenyl methane dyes – phthalein dyes – Xanthene dyes – acridine dyes – sulphur dyes. Phthalocyanines –Cyanine dyes. Malachite green, para-rosoaniline, crystal violet.

### Unit V: Pigments

Pigments – requirements of a pigment, organic and inorganic pigments, white pigment – white lead – blue pigment – ultramarine blue – red pigment – red lead – green pigments – chrome green.

Fluorescent brightening agents, Optical brighteners.

### Text Books:

1. B.K. Sharma, M. Sharma, "Industrial Chemistry", 10<sup>th</sup> edition, GOEL Publishers, Meerut, 1999
2. M. G. Arora & M. Singh, "Industrial Chemistry", Anmol Publications Private Ltd., 2002

3. K. Venkataraman, "The Chemistry of synthetic dyes", Vol.I, II, III & IV, Academic Press, N.Y.,1949.

**Reference Books:**

1. The chemistry of synthetic dyes and pigments – H.A.Lubs, ACS publication, Halner,1970
2. I. L. Finar, Organic Chemistry, Vol.2, ELBS 5<sup>th</sup> Edition, 1989

## CH346 TEXTILE PROCESSING

**Credits:4:0:0**

### Unit I : Fibre Science

Fibre characteristics and their influence on textile products – general classification of fibres natural and man made fibres – identification of textile fibres – burning test, microscopic appearance and chemical test methods.

### Unit II: Preparatory Processes

Chemistry and practice of preparatory processes for cotton – desizing, scouring, bleaching, mercerization of cotton - carbonization, bleaching of wool -degumming, bleaching of silk. Preparatory processes for nylon, polyester and acrylic and polyester/cotton-blends.

### Unit III: Dyeing

Classification of dyes – application and structure, Theory of dyeing – dye fibre interaction, Dyeing of cotton - reactive and vat dyes, wool – acid, basic dyes, silk –acid, basic dyes, polyester – disperse dyes. Methods for determination of wash, light and rubbing fastness. Evaluation of fastness properties with grey scale.

### Unit IV: Printing

Styles of printing. Ingredients of Printing paste, Printing of cotton with reactive dyes. Printing of wool, silk, nylon with acid and metal complex dyes. Printing of polyester with disperse dyes. Methods of dye fixation after printing. Transfer printing of polyester, Battick printing (Tie and dye), Flock printing, Foam printing, bubble printing.

### Unit V: Finishing

Mechanical finishing of cotton - Starch finish, Wrinkle resistant, water repellent, flame retardant and enzyme (bio-polishing) finishing of cotton. Milling, and shrink resistant finishing of wool. Antistatic finishing of synthetic fibre fabrics. Heat setting of polyester.

**Text books:**

1. V.A. Shenai, "Technology of textile processing", Sevak publications, 1971
2. Marsh J.T, "Textile Science – An Introductory Manual", B.I. Publications, 1979

**Reference Books:**

1. A. A. Vaidya, Production of synthetic fibres, Wiley-Interscience, 1984
2. H.B. Marcel Dekker "Handbook of Fiber Science & Technology", Textile Institute, Manchester, Vol. 3, 1998.

## CH347 CHEMISTRY AND PROCESSING OF ELECTROCERAMICS

**Credits:4:0:0**

### **Unit I. Basics of material science**

Crystal structure and characterization of materials, Bragg's law, X ray diffraction - Crystal imperfections - Electrical properties of materials, resistivity, conductivity, semiconductors: intrinsic/extrinsic semiconductors, insulating materials, dielectric materials, piezoelectricity - Magnetic properties of materials, classification of magnetic materials, description - Diffusion in solids, fick's law.

### **Unit II. Synthesis of ceramic powders**

Preparation of ceramic powders – Alumina, Zirconia, Perovskites and spinels - solid state reaction – solution processes - sol gel processing – combustion synthesis technology- vapour-phase reactions

### **Unit III. Ceramic powder characterization**

Powder Characterization - Physical characterization - Types of particles, particle size measurement – sieving – sedimentation - light scattering - electrical sensing zone technique (the coulter counter) - x-ray broadening - surface area – porosity (gas absorption, mercury porosimeter, pycnometry) - chemical composition; bulk composition - surface characterization- Scanning Electron Microscopy, Transmission Electron Microscopy

### **Unit IV. Ceramic Processing**

Fabrication of components – Role of binders, plasticizers, lubricants, deflocculates and flocculants as processing aids - shaping techniques such as powder compaction, extrusion, injection moldings, slip casting, screen printing & tape casting – characterization – Thermogravimetric / differential thermal analysis - solid state and liquid phase sintering

### **Unit V. Applications of Electroceramics**

Capacitors – Ceramic sensors - Resistors – Varistors – Thermistors – Electrochemical devices – Fuel cells - Batteries

### **Text books:**

1. K.J. Rao, "Perspectives in Solid State Chemistry", Narosa and Wiley Publishers, 1995
2. R.E. Smallman and R J Bishop, "Metals and Materials -Science, Processes, Applications", Butterworth-Heinemann, Oxford, 1995
3. M.N.Rahaman, "Ceramic Processing and Sintering", Marcel Dekker, Inc., New York, 1995
4. J.S. Reed, "Principles of Ceramic Processing", John Wiley & Sons, Inc., New York, 1995
5. R.C. Buchanan, "Ceramic Materials for Electronics", Marcel Dekker, New York, 1986
6. W. David Kingery, H. K. Bowen, and Donald R. Uhlmann, "Introduction to Ceramics", 2<sup>nd</sup> edition, from Wiley-Interscience, 1976

**Reference books:**

1. Powder Metallurgy, Metals Hand Book, 9<sup>th</sup> edition, Vol. 7, ASM International, 1994
2. D.W. Richerson, "Modern Ceramic Engineering", 2nd ed., Marcel Dekker, New York, 1992

**CH348 ADVANCED SPECTROSCOPY****Credit 4:0:0****Unit I - NMR Spectroscopy**

Proton NMR – Instrumentation - Spin of nuclei - chemical shift - Factors affecting chemical shift-Relaxation mechanisms of nuclei - Mechanisms of spin-spin coupling - C<sup>13</sup> NMR - chemical shift correlation – quantitative measurement in C<sup>13</sup> NMR – shift reagents – intensity standards – Decoupled spectra – Off-resonance decoupling

**Unit II - 2D NMR Spectroscopy**

The INEPT experiment – recording and processing of 2D spectrum – COSY methods and principles – hetero-nuclear correlation spectroscopy – HSQC and HMQC – long range correlation – TOSCY – NOE – transient NOE experiment – steady-state NOE experiment – ROESY –Instrumentation, principles and applications  
Principles and applications of solid state NMR – concept of magic angle spinning – TROSY (Transverse Relaxation Optimized Spectroscopy) – use of liquid crystals in TROSY

**Unit III - Mass spectrometry**

Use of mass spectrometry in the structural elucidation of organic compounds – mass spectra of compound containing different functional groups – theory, instrumentation, and application – Atmospheric Pressure Chemical Ionization (APCI) – Electron Spray Ionization Techniques (ESIT) – MALDI techniques for protein analysis – time of flight – LC/MS, LC/(MS)<sup>n</sup>

**Unit IV - Fluorescence Spectroscopy**

Principles of steady state and time-resolved fluorescence spectroscopy – static and dynamic quenching of fluorescence – excited state intra-molecular proton transfer (ESIPT) – intra-molecular charge transfer – calculation of excited state pK<sub>a</sub> values – fluorescence resonance energy transfer (FRET) – fluorescence in-situ hybridization (FISH) – fluorescence recovery after photo-bleaching (FRAP) – fluorescence correlation spectroscopy – fluorescence confocal microscopy – instrumentation, principles and applications of the above methods

**Unit V - Photoelectron, Mössbauer, and ESR Spectroscopy**

Photoelectron spectroscopy, X-ray emission spectroscopy, Mössbauer spectroscopy – principles – spectrometer – isomer shift – quadrupolar interaction – nuclear Zeeman splitting – hyperfine interactions – Electron Spectroscopy for Chemical Analysis (ESCA) - applications

ESR theory – derivative curves – g shift – hyperfine splitting – isotropic and anisotropic systems – zero field splitting and Kramer degeneracy – identification of free radicals – application to copper complexes

**References:**

1. Gurdeep R. Chatwal & Sham K.Anand, *Spectroscopy*, Himalaya Publishing House Mumbai (2004).

2. Gupta Kumar & Sharma, *Elements of Spectroscopy*, Pragati Prakasan, Meerut (2001).
3. P.S.Kalsi, *Spectroscopy of Organic Compounds*, 6th Edition, New Age International Publishers, New Delhi (2004).
4. B.P. Straughan & S.Walker, *Spectroscopy*, John Wiley and Sons, New York (1976).
5. Y.R.Sharma, *Elements of Organic Spectroscopy*, S.Chand & Company Ltd., New Delhi (2004).
6. Colin N. Banwell & Elaine M. Mccash, *Fundamentals of Molecular Spectroscopy*, 4<sup>th</sup> Edition, McGraw-Hill, New Delhi (2004).
7. Jag Mohan, *Organic Spectroscopy Principles and Applications*, Narose Publishing House, New Delhi (2001).
8. D.N.Satya Narayana, *Vibrational Spectroscopy Theory and Applications*, New Age International Publishers, New Delhi (2004).
9. Robert M.Silverstein & Francis X. Webster, *Spectroscopy of Organic Compounds*, 6<sup>th</sup> Edition, Wiley Publications (1998).
10. Russell S. Drago, *Physical Methods in Inorganic Chemistry*, Reinhold Publishing Corporation, New York (1965)
11. Gordon M. Barrow, *Introduction to molecular spectroscopy*, McGraw-Hill, New York, 1962
12. W.Kemp, *Organic Spectroscopy*, 3<sup>rd</sup> Edition, ELBS, 1991
13. H.A.Willard, L.L.Merrit, J.A.Dean, *Instrumental methods of analysis*, Van Nonstrand, New York, 1986
14. Douglas A. Skoog, Donald M. West, F. James Holler, *Analytical chemistry: an introduction*, Saunders, College publications, New York, 1990
15. Dudley H. Williams, Ian Fleming, *Spectroscopic methods in Organic Chemistry*, McGraw- Hill, 1995

### **CH349 MEDICINAL CHEMISTRY**

**Credit 4:0:0**

#### **Unit I - Basics of medicinal chemistry**

Brief history of medicinal chemistry – classification of drugs – brief description of biological, chemical, computer revolutions in drug design – pro drugs and soft drugs – design of pro drug system – multiple pro drug formation – soft drug principle and applications

#### **Unit II - Drug targets and drug solubility**

Enzymes and enzyme inhibitors – competitive and non-competitive inhibitors – reversible and irreversible inhibitors – ligand-receptor theories – Clark's theory and Paton's rate theory – proteins, lipids, and nucleic acids as drug targets – effect of pH, pK<sub>a</sub>, and polarity on drug solubility

#### **Unit III - Pharmacokinetics and drug metabolism**

Natural resources of lead compounds – absorption, distribution, metabolism, and elimination – oxidation and hydrolysis – testing drugs in vitro – high-throughput screening – testing drugs in vivo – therapeutic index and therapeutic ratio

#### **Unit IV - Clinical testing and synthesis of drugs**

Various phases in preclinical testing and clinical trials – designing organic synthesis – convergent synthesis – patenting and manufacture – complexes and chelating agents – metal clusters – detoxification – drug action and metal chelation

### **Unit V - Development of new drugs**

Five classic steps in the design of a new drug – procedures in drug design – isolation of bioactive compounds – accidental discovery – examination of metabolites – interference with fundamental life processes – exploitation of side effects of drugs - random screening – molecular modification of lead compounds – factors affecting drug development

### **References**

1. Foye's *Principles of Medicinal Chemistry*, 5th edition; David A. Williams, William O. Foye, Thomas L. Lemke; Lippincott Williams & Wilkins: Philadelphia, 2002.
2. Wilson and Gisvold's *Textbook of Organic Medicinal and Pharmaceutical Chemistry*, 11th edition; Delgado & Remers, Eds.; Lippincott Williams & Wilkins: Philadelphia, 2004 ("W&G").
3. Burger's *Medicinal Chemistry*, 6<sup>th</sup> ed., Vol. 1-6; D.J. Abraham, Ed. (RS403 .B8 2003 - vol.1-6)
4. *Organic Chemistry of Drug Synthesis*, Vol. I-6, Daniel Lednicer and Lester A. Mitscher (RS 403.L38-vol. 1-6)
5. Goodman & Gilman's *the Pharmacological Basis of Therapeutics*, 10<sup>th</sup> ed., Joel G. Hardman & Lee L. Limbird, Eds.; Alfred Gilman, Contrib. Ed (RM300 .G644 2001

## **CH350 NANOCHEMISTRY**

**Credit 4:0:0**

### **Unit I - Nanochemistry Basics**

Introduction and brief history of nanotechnology – materials vs. molecular self-assembly – ionic, dipolar, hydrogen-bonding,  $\pi$ -bonding, van der Waals and hydrophobic interactions and their significance in nanotechnology – Preparation techniques – evaporation / sputtering, chemical processes, CVD, sol-gel processes, Langmuir-Blodgett film, growth techniques, photolithography, properties and applications of thin and LB films

### **Unit II - Experimental techniques**

Instrumentation, working principle, and applications of scanning electron microscope, transmission electron microscope, scanning tunneling microscope, atomic force microscope, and surface plasmon resonance – theories and principles of soft lithography, self assembled monolayers and multilayers

### **Unit III - Nanomaterials**

Classification, preparation, and properties of metals, bimetallic collids, nano alloys, shape memory alloys, metal oxides, chalcogenides and carbon nanomaterials, nanorods, nanotubes, and nanowires – applications of the above

### **Unit IV - Microporous and mesoporous materials**

Microporous materials, mesoporous materials – block-copolymers – assembling inorganic polymers – molecular switches – fullerenes, calixarenes, dendrimers, cyclodextrins, zeolites, clays, and metalloporphyrins as catalysts

### **Unit V - Nanochemistry in Biological systems**

Nanochemistry in biology and medicine – biomolecular motors and nanomachines – kinesin – bioinspiration in materials design – virus, bacteria, and DNA as bioinspirators – toxicity of nanoparticles – NanoDrug delivery

#### **References:**

1. Jahn Marie Lehn (1993). "*Supramolecular chemistry*". *Science* 260 (5115): 1762–3
2. Gustavo Luengo, Samuel Campbell, Vojislav Srdanov, Fred Wudl, Jacob Israelachvili. *Chemistry of Materials* 9 (1997) 1166–1171
3. S. Chiruvolu, J. Israelachvili, D. Leckband, F-J Schmitt, S. Walker, J. Zasadzinski, *Science* 264 (1994) 1753–1756
4. G.B.Sergeev, *Nanochemistry*, Elsevier Publishers (2005)
5. Jonathan Steed and Jerry Atwood – *Core Concepts in Supramolecular Chemistry and Nanochemistry*, Wiley Publishers (2006)
6. <http://www.uaf.edu/chem/rfk/nano.html>
7. Catherine BrÄchignac, Philippe Houdy, Marcel Lahmani , *Nanomaterials and Nanochemistry*, Springer; 1 edition (February 2008)

## **CH351 GREEN CHEMISTRY**

**Credit 4:0:0**

### **Unit I - Introduction to green chemical principles**

Definition, tools, and twelve principles of green chemistry, solvent-less reactions and reactions in water, microwaves and fluorosolvents, green resolution of racemic mixtures, materials for a sustainable economy, chemistry of longer wear, agrochemicals: problems and green alternate solutions

### **Unit II - Atom efficient processes**

Atom efficient processes, evaluating chemical reagents according to their yield and atom efficiency, examples of efficient stoichiometric and catalytic processes, atom economy and homogeneous catalysis, halide-free synthesis and alternatives to Strecker synthesis

### **Unit III - Greener reagents and products**

Greener solvents – the use of volatile organic compounds and the need for innocuous replacements – use of ionic liquids - the use of supercritical CO<sub>2</sub> – solvent-less, solid-supported reagents, and aqueous systems as alternative solvents - greener reagents and products, avoidance of toxic functional groups, minimizing bioavailability and use of auxiliary materials, examples of greener reagents including replacement of phosgene, solid state polymerizations, alternative nitrile synthesis

### **Unit IV - Renewable resources**

Use of renewable materials, evaluating feedstock and starting materials and their origins, toxicity, sustainability and the downstream implications of the choice of feedstock, commodity chemicals from glucose and biomass conversion

### **Unit V - Catalysis in green chemistry**

Catalysis, energy requirements and usage, optimization of the reaction by minimizing the energy requirements, examples of efficient catalytic reactions including the use of heterogeneous catalysis, zeolites, oxidation using molecular oxygen

#### **References:**

1. Anastas, P. T.; Warner, J. C. *Green Chemistry: Theory and Practice*. Oxford Univ. Press: Oxford, 1998.
2. Matlack, A. S. *Introduction to Green Chemistry*. Marcel Dekker: New York, 2001.
3. [http://www.chemicalstrategies.org/other\\_green.htm](http://www.chemicalstrategies.org/other_green.htm)
4. Mukesh Doble, *Green Chemistry and Engineering*, Academic Press; 1 edition 2007

## **CH352 RECENT ADVANCES IN CHEMISTRY**

**Credit 4:0:0**

### **Unit I - Recent trends in synthetic chemistry**

Olefin metathesis – microwaves as tools for organic synthesis – micro-fluidic closed loops – micro-reactors as tools for synthesis – combinatorial synthesis – carbon nanostructures towards materials for molecular electronics – modern surface chemistry – fuel cells, artificial fertilizers and clean exhaust

### **Unit II - Identification and quantification of phytochemicals**

Identification and quantification of bio-active marker compounds by uv-visible, GC and HPLC methods – identification of anti-oxidants by LC-MS and LC/MS/MS techniques – identification of phytochemicals by APCI-MS, ESI-MS, MALDI, TOF mass spectroscopic techniques – quality control of raw drugs and finished products in the herbal industry

### **Unit III - Phytochemical analysis**

Finger printing of phytochemical extracts by TLC, GC, HPLC – different types of extraction: sequential extraction, extraction using carbon dioxide, hydrodistillation, steam distillation – extraction and analysis of anti-oxidants (flavonoids, isoflavonoids, coumarins and phenolic compounds by spectral methods – determination of anti-oxidant activity by different methods – DPPH, NO, superoxide methods – estimation of phenolic content in an extract – analysis of pesticides, aflatoxins, heavy metals in herbal and food products

### **Unit IV - Unsolved problems and questions of the 21<sup>st</sup> century**

Unsolved problems in chemistry: solvolysis of norbornyl cation, on-water reactions, bond rotation barrier, alpha effect – origin of homochirality in amino acids and sugars, protein folding problem, abiogenesis – hypervalent molecules, water cluster

Questions of the 21<sup>st</sup> century: Can we selectively shut off immune response? How hot the green house world would be? Is an effective HIV vaccine feasible? How far can we push

chemical self-assembly? How are memories stored and retrieved? How much can human lifespan be extended?

Emerging infectious diseases in the 21<sup>st</sup> century

### **Unit V - Indian pharmaceutical industry**

Pharmaceutical industry in India, milestones in the development of pharmaceutical industry, current status and its role in national economy and national health

Structure of the industry, organized sector, small sector, manufacture of pharmaceuticals in public sector

Progress in the manufacture of basic drugs – synthetic and vegetable origin

Export and import of drugs and pharmaceuticals

Various types of insurances including marine insurance

### **References:**

1. [www.sciencemag.org/cgi/content/full/](http://www.sciencemag.org/cgi/content/full/)
2. [www.nano.tu-dresden.de/pages/admo/book/](http://www.nano.tu-dresden.de/pages/admo/book/)
3. Rakesh Parashar, *Reaction mechanisms in organic synthesis*, Blackwell publishers
4. [www.tan-delta.com](http://www.tan-delta.com)
5. K. Kwok, J. K. Ellenbogen, *Moletronics: future electronics*, Materials today 2005, volume 5, pages 28 – 37
6. M. C. Petty, M. R. Bryce, D. Bloor, *Introduction to molecular electronics*, Oxford University press, New York
7. N. Shakuntala Manay, N. Shadhiksharawamis *Food: facts and principles*, CEM Publishing
8. Brittany L. Hayes, *Microwave synthesis*, CEM publishing
9. [http://mpira.ub.uni-muenchen.de/8144/1/MPRA\\_paper\\_8144.pdf](http://mpira.ub.uni-muenchen.de/8144/1/MPRA_paper_8144.pdf)

## **CH353 SUPRAMOLECULAR CHEMISTRY**

**Credit 4:0:0**

### **Unit I - Introduction**

Supramolecular chemistry – introduction - the lock and key principle and induced-fit model – co-operativity and chelate effect – pre-organization – binding constants – kinetic and thermodynamic selectivity – ionic and dipolar interactions – hydrogen bonding – pi-interactions – van der Waals interactions – hydrophobic effects

### **Unit II - Solution host – guest chemistry**

Cation binding – crown ethers and cryptands – spherends, hemispherends, heterocrowns, and heterocryptands – Schiff's bases – calixarenes – biological ligands: ion channels and siderphores

Anion binding – charged receptors, neutral receptors, Lewis-acid receptors and anti-crowns – metal-containing receptors

Neutral molecule binding – cyclophane hosts – carcerands and hemicarands – cyclodextrins – clefts and tweezers

### **Unit III - Rotoxanes, catenanes, and knots**

Molecular polygons – rotoxanes, catenanes, and knots – template synthesis of rotoxanes – threading, trapping, clipping, and slipping – borromeates – molecular containers – metal-directed capsules – hydrogen-bonded capsules

#### **Unit IV - Solid state supramolecular chemistry**

Zeolites – structure, composition, and catalysis – clathrates – urea / thiourea clathrates – trimesic acid clathrates – hydroquinone and Dianin's compound – crystal engineering – the Cambridge structural database – crystal engineering with hydrogen bonds – metal-organic frameworks

#### **Unit V - Molecular devices**

Molecular devices – photochemical devices – molecular wires and rectifiers – molecular switches – molecular muscles – structure and properties surfactants, micelles, and vesicles – liquid crystals – dendrimers – fibres, gels, and polymers – supramolecular gels

#### **References:**

1. Jahn Marie Lehn (1993). "Supramolecular chemistry". *Science* 260 (5115): 1762–3
2. J. –M. Lehn, *Supramolecular Chemistry*, Wiley-VCH (1995) ISBN-13:978-3527293117
3. Gustavo Luengo, Samuel Campbell, Vojislav Srdanov, Fred Wudl, Jacob Israelachvili. *Chemistry of Materials* 9 (1997) 1166–1171
4. S. Chiruvolu, J. Israelachvili, D. Leckband, F-J Schmitt, S. Walker, J. Zasadzinski, *Science* 264 (1994) 1753–1756
5. Jackie Ying - <http://www.hindawi.com/70382969.html>
6. Jonathan Steed and Jerry Atwood – *Core Concepts in Supramolecular Chemistry and Nanochmistry*, Wiley Publishers (2006)
7. <http://www.uaf.edu/chem/rfk/nano.htm>

## **CH354 CORROSION SCIENCE AND ENGINEERING**

**Credit 4:0:0**

### **Unit I - Introduction to corrosion**

Definition - Classification and economics of corrosion - Faraday's law - Nernst equation - emf and galvanic series - potential-pH diagram for Fe-H<sub>2</sub>O system - mixed potential theory - activation and diffusion controlled corrosion processes – passivation - principle of potentiostatic and galvanostatic techniques.

### **Unit II - Types of corrosion**

Types of corrosion - Influencing factors and corrosion control methods for various forms of corrosion – pitting corrosion - inter granular corrosion – crevice corrosion – decarburization – dezincification - stress corrosion cracking - fretting corrosion - corrosion processes and control methods in fertilizers, petrochemical, paper and sugar industries.

### **Unit III - Mechanisms of corrosion**

Atmospheric corrosion – classification - Pilling-Bedworth rule - factors influencing atmospheric corrosion - wet corrosion - factors influencing wet corrosion - mechanism of marine corrosion - pipeline corrosion - biologically induced corrosion.

#### **Unit IV - Corrosion monitoring and testing**

Monitoring and laboratory analysis of corrosion rates - short term and long term accelerated tests for studying different forms of corrosion - measurement of corrosion rate by physicochemical and electrochemical techniques.

#### **Unit V - Methods of corrosion control**

Cathodic protection – anodic protection - corrosion inhibitors for acidic, near neutral and alkaline media - corrosion inhibitors for cooling water and boiling water systems - Langelier saturation index.

#### **References:**

1. Raj Narayanan, 'An Introduction to metallic corrosion, Oxford and IBH, 1983
2. S.N. Banerjee, 'An introduction to corrosion and corrosion inhibition' Oxonian Press Ltd, New Delhi.
3. M.G.Fontana and N.D.Greene, 'Corrosion Engineering,, McGraw Hill, New York
4. H.H.Uhlig, 'Corrosion and corrosion control', A Wiley Inter science publication, John Wiley & sons, New York.
5. Chamblairlain J and Tretheway K.R, "Corrosion for Science and Engineering", 2<sup>nd</sup> edn. Longman Scientific & Technical, England, 1995.

**ADDITIONAL SUBJECTS**

| <b>Code</b> | <b>Name of the Subject</b>                      | <b>Credit</b> |
|-------------|---|---------------|
| 09CH104     | Applied Chemistry Lab                           | 0 : 0 : 2     |
| 09CH201     | Environmental Studies                           | 3 : 0 : 0     |
| 09CH355     | Chemistry Lab for Physicists                    | 0 : 0 : 2     |
| 09CH356     | Colloid Chemistry and Liquid crystals           | 4:0:0         |
| 09CH357     | Environmental Electrochemistry                  | 4:0:0         |
| 09CH358     | Electro organic synthesis                       | 4:0:0         |
| 09CH359     | Advanced Electro Chemistry                      | 4:0:0         |
| 09CH360     | Electro Analytical Chemistry                    | 4:0:0         |
| 09CH361     | Materials Electro Chemistry                     | 4:0:0         |
| 09CH362     | Electrodeposition Techniques                    | 4:0:0         |
| 09CH363     | Chemistry of Energy Sources and Storage Devices | 4:0:0         |
| 09CH364     | Organic Chemistry                               | 4:0:0         |
| 09CH365     | Research Methodology in Chemistry               | 4:0:0         |

**09CH104 – APPLIED CHEMISTRY LAB****Credit 0:0:2****Objectives:**

1. To understand the principles of estimation in acidimetry, alkalimetry and permanagnometry titrations
2. To understand gravimetric principles involved in complexometric titration
3. To understand the principles of potentiometry, conductometry and pH measurements
4. To understand the principles of spectrophotometry and flame photometry

**List of Experiments:**

1. Estimation of Hydrochloric acid
2. Estimation of Sodium Hydroxide
3. Estimation Fe<sup>2+</sup> ions
4. Estimation of total, permanent and temporary hardness of Water Sample
5. Estimation of alkalinity in water sample
6. Estimation of dissolved oxygen
7. Estimation of Iron in water sample by spectrophotometry
8. pH measuremnts for acid – alkali titration

9. Conductometric estimation of an acid
10. Potentiometric estimation of  $\text{Fe}^{2+}$  Ions
11. Determination of single electrode potential by potentiometry
12. Determination of rate of corrosion of mild steel by weight loss method
13. Estimation of sodium present in water by flame photometry

### Reference Books

1. G.H. Jeffery, J. Bassett, J. Mendham and R.C. Denney, "Vogel's text book of quantitative chemical analysis", ELBS, 6<sup>th</sup> Edition, Longman, Singapore publishers, Singapore, 2004
2. I.M. Kolthoff and E.B. Sandell, "Quantitative Chemical Analysis" MacMillan, Chennai, 1980
3. S.K. Bhasin and S.K. Sudha Rani, "Laboratory Manual on Engineering Chemistry", Dhanpat Rai Publishing Company (P) Ltd., 2003

## 09CH201 – ENVIRONMENTAL STUDIES

**Credit 3:0:0**

### Objectives:

1. To acquire the knowledge of environmental studies, its need & importance
2. To understand the concept, structure and function of different ecosystems
3. To know about pollution problems and green technology
4. To develop a sense of responsibility about the role of students in fostering the idea of learning to live in harmony with nature

### Unit I - Natural resources, ecosystems and biodiversity

Environment - Definition, scope and importance – Forest resources: Use and overexploitation, Water resources: Use and over-utilization, dams-benefits and problems – Energy resources: Growing energy needs, renewable and non renewable energy sources, use of alternate energy sources – Land resources: land degradation – Role of an individual in conservation of natural resources Ecosystem – Structure and function – Ecological succession – Introduction to various ecosystems. Biodiversity – Definition and types – Threats to Biodiversity in India and its impacts – Conservation of Biodiversity: In-situ and Ex-situ conservation of biodiversity

### Unit II – Air pollution and global issues

Air pollution - Introduction – atmospheric constituents – Chemical reaction in the atmosphere – air pollutants – classification – effects on human, animal, plant, property and environment – control methods for particulates and gaseous pollutants – control of pollutants from automobiles – Burning of plastics – PCBs and their impact - Green house gases – Photochemical reaction – green house effects - climate change - global warming and its effects – international climate conventions, protocols and perspectives – technology and policy options for GHG emission mitigation - acid rain, ozone layer depletion and solutions

**Unit III – Issues related to other environmental pollution aspects and green technology**

Water pollution - sources – characteristics – BOD, COD - pollutants and their effects – heavy metal pollution – inorganic and organic pollutants control methods - Advanced waste water treatment techniques - Basic aspects of soil pollution - marine pollution - noise pollution - thermal pollution - nuclear hazards - Causes, effects and control measures - solid waste management: causes, effects and control measures of urban and industrial solid wastes

Green chemistry and green technology – principles of sustainable and green chemistry - miscelle templated silica as catalyst in green chemistry – biocatalysis – bioproduction of catalysts in industries – basics of clean energy technology for the future – fuel cells, wind power, solar power

**Unit IV – Environmental Legislation**

Pollution controls acts – environment protection act – water pollution act – air pollution act – wildlife (protection) act, 1972 – forest (conservation) act, 1980 – polluter pays principle – precautionary principle – Issues in pollution control enforcement and public awareness – issues of environment – public awareness

**Unit V - social issues and the environment**

From Unsustainable to Sustainable development – Urban problems related to energy – Water conservation, rain water harvesting, watershed management - Population growth, variation among nations – Population explosion – Environment and human health – Role of Information Technology in Environment and human health – Family welfare programme – HIV / AIDS – women and child welfare – Disaster management: floods, earthquake, cyclone and landslides

**Text books:**

1. Deeksha Dave and S.S. Katewa, “Textbook of Environmental studies”, Cengage Learning, 2008
2. Deswal S and Deswal A, ‘A basic course in Environmental studies’, Dhanpat Rai & Co, First edition, Delhi, 2004
3. Kurian Joseph and Nagendran R, ‘Essentials of Environmental studies’, Pearson Education Pvt Ltd., First edition, Delhi, 2004
4. Santhosh Kumar Garg, Rajeswari Garg and Ranjani Garg, ‘Environmental Science and Ecological Studies’, Khanna Publishers, Second Edition, New Delhi, 2007.

**Reference books:**

1. Gilbert M.Masters, ‘Introduction to Environmental Engineering and Science’, Pearson Education Pvt. Ltd., Second Edition, 2004.
2. Tivedi R.K., ‘Handbook of Environmental Laws, Rules, Guidelines, Compliances and Standards, Vol. I and II, Enviro Media., 1998
3. Cunningham, W.P.Cooper, T.H.Gorhani, ‘Environmental Encyclopedia’, Jaico Publ., House, Mumbai, 2001.
4. Wager K.D., ‘Environmental Management,’ W.B. Saunders Co., Philadelphia, USA, 1998.
5. James Clark & Duncan Macquarie, “Green Chemistry & Technology”, Blackwell publishing, 2002

**09CH355 – CHEMISTRY LAB FOR PHYSICISTS****Credit 0:0:2****Objectives:**

1. To know the method of preparing solutions with different concentrations
2. To understand the volumetric analysis and to understand the method of finding the strength of unknown solutions
3. To understand gravimetric analysis and to estimate the cations like silver and barium from their salts AgCl and BaCl<sub>2</sub> by gravimetric analysis
4. To understand potentiometry, conductometry and pH measurements

**List of Experiments:**

1. Preparation of standard solutions – Normal, Molar and Molal solutions
2. To find out the strength of a given potassium permanganate (KMnO<sub>4</sub>) solution by titrating against N/20 standard mohr's salt (FeSO<sub>4</sub>. (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>. 6 H<sub>2</sub>O) solution
3. Determination of strength of a given solution of K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> solution provided with ferrous ammonium sulphate solution and N-phenyl anthranilic acid solution as an internal indicator
4. To determine the strength of a given copper sulphate solution with N/20 sodium thiosulphate (hypo) solution
5. To determine the Ferrous (Fe<sup>2+</sup>) and Ferric (Fe<sup>3+</sup>) ions in a given solution of iron ore by KMnO<sub>4</sub> method
6. Estimation of Nickel using Eriochrome Black – T indicator
7. Determination of Copper by Complexometric titration
8. Determination of total hardness of water by EDTA method
9. Estimation of barium as barium chloride
10. Estimation of silver as silver chloride
11. To find out the normality of hydrochloric acid solution (N/10) by titrating it against sodium hydroxide solution conductometrically
12. To find out the percentage purity of AgNO<sub>3</sub> solution conductometrically, using N/10 KCl solution.
13. Determine the molarity of HCl by pH-metrically, provided M/10 NaOH
14. To estimate the strength of give hydrochloric acid solution by titrating against sodium hydroxide solution (0.1 N) using quinhydrone as the indicator electrode

**Reference Books**

- 1 G.H. Jeffery, J. Bassett, J. Mendham and R.C. Denney, "Vogel's text book of quantitative chemical analysis", ELBS, 6<sup>th</sup> Edition, Longman, Singapore publishers, Singapore, 2004
- 2 I.M. Kolthoff and E.B. Sandell, "Quantitative Chemical Analysis" MacMillan, Chennai, 1980
- 3 G.Svehla, "Vogel's Qualitative Inorganic Analysis", 6<sup>th</sup> Edn., Orient Longman, New Delhi, 1987

4. S.K. Bhasin and S.K. Sudha Rani, "Laboratory Manual on Engineering Chemistry", Dhanpat Rai Publishing Company (P) Ltd., 2003

## **09CH356 - COLLOID CHEMISTRY AND LIQUID CRYSTALS**

**Credit 4:0:0**

### **Objectives:**

1. To study about surfactants and colloidal systems
2. To understand the rheology of micellar systems
3. To study about liquid crystals and their applications

### **Unit I - Physical Chemistry of interfaces**

Surface chemistry – adsorption by solids – the state of adsorbed molecules – The langmuir theory of adsorption – B.E.T. theory of multilayer adsorption – types of adsorption isotherms – adsorption from solutions – the Gibbs adsorption isotherm for adsorption from solutions – Insoluble surface films on liquids – adsorption chromatography

### **Unit II - Surfactants and colloids**

Surfactants - Classification, cationic, anionic zwitterionic surfactants, Applications. Solubilisation phenomena, Electrophoresis. Electro-osmosis. Dialysis, electro dialysis Ultrafiltration in surfactant systems - Critical micellar concentration and its determination. Classification of colloids, Lyophobic and Lyophilic sols, size and range. Associated colloids, Micelles, Micellar size, shape, character Structure, Spherical rod-like hexagonal and Worm like micelles, Vesicles, classification, Light scattering and Cryo-TEM studies of vesicles. Preparation and purification of colloidal systems, stability of colloids. Thermo Tunable Fluids, Photo tunable Fluids, Magneto and Electro Tunable Fluids.

### **Unit III - Rheology of Micellar Systems**

Introduction to rheology, Newtonian fluids, Shear thinning and shear thickening fluids, Polymers and plastics, Rheology of worm like micelles and vesicles, Rheology models, Application of models in to rheology of micelles mixed micelles and vesicles

### **Unit IV - Liquid Crystals – I**

Introduction of different types of liquid crystals; Symmetry, textures, microscopic and optical properties of different types of nematic, smectic and cholesteric liquid crystal; Blue phases; Electrical and dielectric properties of liquid crystal; Chiral liquid crystals; Ferroelectric liquid crystals; Electro-optic and magneto-optic effect of liquid crystals

### **Unit V - Liquid Crystals - II**

Lyotropic liquid crystals, formation and stability, Differential Scanning Calorimetric and x-ray spectroscopy studies of liquid crystals, liquid crystal displays, Photonic crystals, Optical

switching devices, Optical Limiting Properties of Colloidal Crystals, memory devices; Applications of liquid crystals.

**Text Books:**

1. D. J. Shaw, "Introduction to Colloid and Surface Chemistry", Fourth Edition, Butterworth/Heinemann, Oxford, 1992
2. Paul C. Hiemenz and Raj Rajagopalan, "Principles of colloid and surface chemistry", Marcel Dekker, 1997

**Reference Books:**

1. M.J. Rosen, "Surfactants and interfacial phenomena", Wiley, New York, 1978.
2. J.H Fendler and E.J Fendler, Catalysis in Micellar and Macromolecular Systems, Academic Press, New York, 1975.
3. Prince L.M Edition, "Micro Emulsion", Academic Press, New York, 2000.
4. Douglas A. Skoog, Donald M. West, F. James Holler and Stanley R. Crouch, "Fundamentals of Analytical Chemistry", (Eight Edition), Thomson Learning Inc, 2005.
5. Michel R. Fisch, "Liquid Crystal Lap Top and Life", World Scientific Vol 23 USA. 2001

**09CH357 - ENVIRONMENTAL ELECTROCHEMISTRY****Credit: 4:0:0**

**Objectives and structure:** This course is aimed at providing the student a solid background on topics linking environmental issues such as environmental phenomena, environmental protection and remediation and manmade environmental damages, with electrochemical phenomena.

The course will be divided into two main parts: In the first part the students will be exposed to basics in electrochemistry and the second part will be devoted to in-depth electrochemically oriented environmental issues.

**Unit I - Principles of electrolyte solutions**

Ion-solvent interactions (Born Model, Ion-Dipole model), ion-ion interactions (Debye-Huckel theory, ionic atmosphere), dielectric constant, the significance of Debye length, the significance of activity coefficient. Ion transport in solutions: Diffusion, random walk, convection, migration under the influence of an electrical field, conductivity, equivalent conductivity; electrophoretic effect.

**Unit II - Reactions at the electrode-solution interface**

The origin of surface charges, the metal –solution interface, the electrical double layer, outer and inner Helmholtz planes, the diffuse double layer, Gouy-Chapman-Stern theory for the structure of the electrical double layer, differential capacitance, ionic strength, the influence of ionic strength on the properties of the interface. Introduction to electrochemical kinetics: Electron transfer through the interface (the Butler-Volmer equations), Tafel equation, ion diffusion at the interface, the entire I-V curve, rate limiting step, special mass transfer cases at the interface.

**Unit III - Interfacial phenomena-related topics**

*Stability of colloidal systems:* classification of colloids, significance of colloids in environmental issues, electrostatic interactions, London-Van der Waals interactions, Born interactions, depletion forces, the DLVO theory, coagulation and flocculation, influence of ionic strength and ionic charge (Schulze–Hardy rule) on stability.

*Electrokinetics:* What happens to the interfacial charge distribution in a flowing solution?, the shear plane (significance of zeta potential), electroosmosis, streaming potential, electrophoresis, sedimentation potential, description by force-flux relation (according to irreversible thermodynamics), Helmholtz-Smoluchowski equation, measuring electrokinetic phenomena, soil remediation by electrokinetic phenomena.

#### **Unit IV - Electrochemical reactors**

Classification of electrochemical reactors, unique features of electrochemical reactors, structure, energy consumption, space-time yield, advantages and disadvantages of electrochemical reactors, special types of electrochemical reactors.

#### **Unit V- Environmentally-related electrochemical issues**

Electrochemical methods for water and wastewater purification- removal of metals, oxidation and reduction of organic contaminants (direct oxidation or reduction, mediated electrochemical oxidation- the CerOx process, ex-situ electrochemical production of oxidizing agents- chlorine, ozone, hydrogen peroxide, ClO<sub>2</sub>), electro dialysis –principles and applications, principles of electrochemical measurements and sensing, fuel cells and bioelectrochemistry for cleaner energy, electrocoagulation.

#### **Text Books**

1. J. Koryta, J. Dvorak, L. Kavan “Principles of Electrochemistry”, John Wiley Publishers, 1993
2. S. Glasstone, *Textbook of Physical Chemistry*, Macmillan, Bombay, India, 2nd edition, 1974.

#### **References**

1. Duncan A MacInnes, “The principles of Electrochemistry”, Reinhold publishing corporation, 1998
2. Bockris & Reddy, “Modern Electrochemistry”, Springer, Volumes 1 & 2, 1973
3. K Scott, “Electrochemical Reaction Engineering”, Academic Press, London 1991
4. P. Delahay, “Double Layer and Electrode Kinetics”, USA: Wiley-Interscience, 1965
5. C. A. C. Sequeira, “Environmental oriented electrochemistry”, Elsevier 1994
6. Christos Comninellis, Marc Doyle, Jack Winnick, “Energy and electrochemical processes for a cleaner environment: proceedings” by Electrochemical Society, International Society of Electrochemistry, Electrochemical society Etats-Unis Energy technology division, Electrochemical Society Meeting. - Science - 2001

**09CH358 - ELECTRO-ORGANIC SYNTHESIS****Credit 4:0:0****Objectives:**

1. To study about synthesis of organic compounds using electrochemistry processes
2. To study about organic electrode processes
3. To study about industrial electroorganic chemistry, electrochemical polymerization and chemically modified electrodes

**Unit – I**

Principles and methods, Synthesis and mechanistic aspects of cathodic reactions of organic compounds classified by electrophores, Hydrocarbons, Nitro and related compounds, Carbonyl compounds.

**Unit – II**

Synthetic and mechanistic aspects of anodic reactions of organic compounds classified by electrophores, Anodic oxidation of hydrocarbon, Carboxylic acids.

**Unit – III**

Electrode reactions classified by reaction type, Reductive coupling, Oxidative coupling, Cleavages and deprotection, Anodic substitution, Anodic fluorination.

**Unit – IV**

Stereochemistry of organic electrode processes, Amalgam and related reductions, Electrogenerated reagents, Electrogenerated acids and bases.

**Unit – V**

Presents and future applications, Industrial electroorganic chemistry, Electrochemical polymerization, Chemically modified electrodes and conducting polymers.

**Text Books:**

1. M.R. Rifi, Covitz and H. Frank, "Introduction to Organic Electrochemistry", ECS Princeton, 1990
2. Sigeru Torri, "Novel trends in Electroorganic Synthesis", Springer, 1998

**Reference Books:**

1. Sergio Trasatti, "Electrodes of Conductive Metallic Oxides". Elsevier Scientific Publishing Company, Amsterdam-Oxford-NY, 1980.
2. Tatsuya Shono, "Electroorganic Chemistry", Academic Press, 1990

**09CH359 - ADVANCED ELECTROCHEMISTRY****Credit 4:0:0****Objectives:**

1. To study about fundamentals of electrochemistry
2. To study about electro-kinetic phenomena
3. To understand electro catalysis

**Unit I - Electrical Double Layer**

Thermodynamics of ideally polarisable and non-polarisable interfaces- Lipman equation- Determination of interfacial tension, Charge density, surface excess.

**Unit II - Double layer capacitance by electro capillary & bridge methods-Helmholtz, Gouy-chapman & Stern models of the double layer Contact adsorption & its determination.**

**Unit III - Electrode Kinetics**

Concepts of equilibrium potential, Nernst equation, over potential & its different types, equilibrium exchange current density- Derivation of Butler Volmer equation-High field & low field approximations

**Unit IV - Charge transfer resistance & polarizability of the interface – concepts of rate determining step, stoichiometric number, reaction order- Determination of step wise mechanism of an electrode reaction- Electro kinetic Phenomena- basic concepts.**

**Unit V - Electro catalysis**

Chemical analysis & Electro catalysis- comparison of Electro catalysis-Electro analysis in simple redox reactions involving adsorbed species-special features of electro catalysis-Discussion on the mechanisms of hydrogen evolution and oxygen reduction reactions.

**Text Books:**

1. D.R. Crow, "Principles and Applications of Electrochemistry", Edition – IV, London, Blackie Academic and Professional, 1994
2. S. Glasstone, "Introduction to Electrochemistry", East-West Press Pvt. Ltd., 1965

**Reference Books:**

1. V.S. Bagotsky, "Fundamentals of Electrochemistry", Wiley-interscience, 2005
2. Paul Delahay, "Double Layer and Electrode Kinetics", Interscience-Wiley, 1965

**09CH360 - ELECTRO ANALYTICAL CHEMISTRY****Credit: 4:0:0****Objectives:**

1. To study about Tafel and linear polarization methods
2. To study about cyclic voltammetry techniques
3. To understand the concept of Faradaic impedance, Nyquist and bode plots

**Unit – I**

Determination of kinetics parameters [ $i_o$ ,  $k_s$ ,  $\beta(\alpha)$ ] by Tafel and linear polarization methods - Ion selective electrodes –selectivity coefficient– amperometric sensing and determination of dissolved oxygen.

**Unit - II**

Linear sweep voltammetry and cyclic voltammetry Derivation of Randles- Sevciks equation – effect of sweep rate-Discussion of reversibility and interpretation of experimental data.

**Unit - III**

Potential step method (chronoamperometry) under diffusion control Derivation of Coettrell equation for a planar and spherical electrode- significance of spherical diffusion – Derivation of Ilkovic equation.

**Unit - IV**

General theory of controlled current methods-Derivation of Sands equation for constant current input under linear diffusion-chrono potentiogram and its significance.

**Unit - V**

Alternating current methods-concepts of Faradaic impedance –derivation of kinetic parameters from impedance measurements – Nyquist and bode plots for simple redox reactions.

**Text Books:**

1. Joseph Wang, “Analytical Electrochemistry”, II Edition, A. John Wiley & Sons, Inc. 2000
2. Plambeck, James A., “Electroanalytical Chemistry - Basic Principles and. Applications”, University of Alberta, John Wiley & Sons, 1982

**Reference Books:**

1. Paul Delahay, "Double Layer and Electrode Kinetics", Interscience-Wiley, 1965
2. B.H.Vassos and G.W.Ewing, “Electroanalytical Chemistry”, John Wiley & Sons, New York, 1983
3. Paul M.S. Monk, “Fundamentals of Electro-Analytical Chemistry”, Wiley, 2001

**09CH361 - MATERIALS ELECTROCHEMISTRY****Credit: 4:0:0****Objectives:**

1. To study about spinel type oxide electrodes
2. To study about electrochemical properties of materials
3. To understand the difunctional mechanism involving reactive surface oxide

**Unit – I**

Properties of Spinel-Type Oxide Electrodes: Crystalline Structure and Preparation, Chemical and Electrochemical Parameters, Chemical, Electrochemical and Adsorption Properties,

**Unit – II**

Properties of Conductive Transition Metal Oxides with Rutile-Type Structure: Physicochemical Properties of Transition Metal Dioxides, Single Crystals, Mixed Oxide Films.

**Unit – III**

Electrochemical Properties of Transition Metal Dioxides, Surface and Intrinsic Redox Properties, Adsorption Properties, electrodic Behavior, Interface: Properties of Oxide Surfaces, adsorption at Gas / Solid Surfaces, Surface Porosity, The Solid / Solution Interface, The Electrical Double Layer at the Oxide / Aqueous Solution Interface,

**Unit – IV**

Reactions of Hydrogen and Organic Substances with and at Anodic Oxide Films at Electrodes: Organic Oxidations with Pt and PbO<sub>2</sub> Anodes, Surface Oxidation of Pt, Mechanisms in Oxidation of H<sub>2</sub> and Organics,

**Unit – V**

Difunctional Mechanism Involving Reactive Surface Oxide, Carbonium-ion Mechanisms, Anodic Reactions of H<sub>2</sub> and Simple Organic Substances at Catalytic Electrode Surfaces, Oxygen and Chlorine Evolution at Conductive Metallic Oxide Anodes: Concepts in Electrocatalysis.

**Text Book**

1. Sergio Trasatti, "Electrodes of Conductive Metallic Oxides", Elsevier Scientific Publishing Company, Amsterdam-Oxford, NY 1980
2. Walfried Plieth, "Electrochemistry for Materials Science", Elsevier Science, 2008

**Reference Book**

1. Paul Delahay, "Double Layer and Electrode Kinetics", Interscience-Wiley, 1965
2. John O'M Bockris, Amulya K. N. Reddu, Maria Gamboa-Aldeco, "Modern Electrochemistry", Kluwer Academic / Plenum Publishers, 2000

## 09CH362 - ELECTRODEPOSITION TECHNIQUES

**Credit: 4:0:0**

### **Objectives:**

1. To study about electrodeposition techniques
2. To study about standard electrode potential and their applications
3. To study the electrodeposition of metals like copper, nickel, chromium, nickel-chromium, etc.

### **Unit - I**

Formation of simple and complex ions – Ions in solutions of electrolytes – Conductivity of solutions – Quantity of electricity and Faraday's laws – Current efficiency

### **Unit - II**

Ionization of water – Significance of pH – Determination of pH values by electrometric methods – Theory of pH indicators – Buffer solutions

### **Unit - III**

Reversible electrode potential – Its significance - Standard electrode potential and their applications – Electrode potentials and the displacement of metals – Deposition potentials of metals

### **Unit – IV**

Hydrogen overvoltage and its importance in metal deposition – Concentration polarization and the diffusion layer – Electrolysis of complex cyanide solutions – Conditions affecting the form of electrodeposited metals – The behaviour of anodes (passivity)

### **Unit – V**

Electrodeposition of copper, nickel, chromium, nickel-chromium, zinc, Alloy deposition – Bath formulation – Process sequence – Deposit analysis – Adhesion, Thickness, Porosity, Hardness, Corrosion resistance – Structural and morphological analysis.

### **Text book:**

1. E. Raub and K. Muller, "Fundamentals of metal deposition", Elsevier, New York 1967
2. Schlesinger, "Modern Electroplating", John Wiley, 2002

### **Reference Books:**

1. N.V.Parthasarathy, "Practical Electroplating Handbook", prentice Hall, Englewood Cliffs, NJ, 1989
2. S. Glasstone, "Introduction to Electrochemistry", East-West Press Pvt. Ltd., 1965

**09CH363 - CHEMISTRY OF ENERGY SOURCES AND STORAGE DEVICES****Credit: 4:0:0****Objectives:**

1. To study about chemical energy sources
2. To study about electrochemical energy storage devices
3. To study the advanced non-conventional energy sources and bio energy

**Unit – I - Chemical energy sources**

Introduction to energy; Fuels – Definition, Classification: Natural and synthetic or (i) Primary – Solid, Liquid and Gaseous fuels and (ii) Secondary – Solid, Liquid and gaseous fuels. Importance of hydrocarbons as fuels. Calorific value – definition, classification – Gross and Net calorific values, units (S.I.). Experimental determination of calorific value of solid / liquid fuels by using Bomb Calorimeter, numerical problems. Petroleum cracking – definition, Fluidized bed catalytic cracking. Reforming of petrol – explanation with reactions. Octane Number, Cetane Number. Knocking – mechanism, prevention of knocking – anti-knocking agents, Unleaded petrol. Synthetic petrol – Bergius process and Fischer Tropsch process. Power alcohol.

**Unit – II - Electrochemical energy storage devices – Battery technology**

Batteries – Introduction, Basic concepts – principal components of a battery operation of a battery during discharge and charge. – Classification of batteries - Primary, Secondary and Reserve batteries with examples - Fuel Cells - Introduction, definition, differences between a battery and a Fuel Cell and advantages - Types of fuel cells – Alkaline fuel cells, solid polymer electrolyt, phosphoric acid fuel cells, molten carbonate fuel cells, fuel cells and solid oxide fuel cells.

**Unit – III - Advanced non-conventional energy sources – I**

Solar Energy - Photovoltaic cells – Introduction, definition, importance. Solar grade silicon. Properties of silicon relevant to photovoltaics, production of solar grade silicon by chemical vapour deposition method and purification by zone reforming. Doping of silicon and working of a PV cell - Tidal Energy– basic principles; tidal power generation systems; advantages and limitations of tidal power generation.

**Unit – IV -Advanced non-conventional energy sources – II**

Wind Energy– basic principles of wind energy conversion; advantages and limitations of wind power generation

Geothermal Energy – Origin and nature of geothermal energy; classification of geothermal resources; advantages and limitations of geothermal power generation

Hydrogen Energy - Production of hydrogen from nonrenewable and renewable primary energy forms - Use of hydrogen as an energy carrier.

**Unit – V- Bio Energy and their advantages**

Biomass and bio-fuels; energy plantation; biogas generation; types of biogas plants; applications of biogas; energy from wastes – Bio-fuels : Types of Bio-fuels - Bio- Ethanol and Bio – Diesel, Production processes and technologies, Bio-fuel applications, Government Policy and Status of Bio fuel technologies in India

**Text Books:**

1. E.M. Goodger, “Alternative Fuels: Chemical Energy Resources”, Macmillan, 1980
2. Clive D.S. Tuck, “Modern Battery Technology”, Ellis Horwood, 1991
3. G. N. Tiwari, M. K. Ghosal, “Renewable Energy Resources: Basic Principles and Applications”, Alpha Science International, 2005
4. Michael D. Brenes, “Biomass and Bioenergy – New Research”, Nova Science Publishers, 2006

**Reference Books:**

1. S A Abbasi and Naseema Abbasi, “Renewable energy sources and their environmental impact”, Prentice Hall of India, 2001
2. G D Rai, ‘Non-conventional sources of energy, Khanna Publishers, 2000
3. J. C. Kuriakose, and J Rajaram, “Chemistry in Engineering and Technology”, Tata Mcraw-Hill Publications Co. Ltd., New Delhi, 1996
4. Leo J. M. J. Blomen, Michael N. Mugerwa, ‘Fuel Cell Systems’ Springer publishers
5. Clive DS Tuch – Modern Battery Technology, Ellis Harwood, New York, 1991

**09CH364 - ORGANIC CHEMISTRY****Credit: 4:0:0****Objectives:**

1. To study about organic reaction mechanism
2. To study about stereochemistry
3. To study about reagents in organic synthesis and supramolecules

**Unit – I Reaction mechanism – I**

Effect of structure and reactivity – Resonance and field effects –Steric effects- Quantitative treatments of the effect of structure and reactivity –LFER- Hammett and Taft equation - Aromaticity – Huckel’s rule – Aromatic systems with electron numbers other than six- annulenes and heteroannulenes – chemistry of fullerenes – Aliphatic nucleophilic substitution – mechanisms –  $S_N^2$ ,  $S_N^1$ , mixed,  $S_N^1$  &  $S_N^2$ ,  $S_N^1$ . SET, neighbouring group mechanism – Reactivity –effect of substrate, attacking nucleophile, leaving group and reaction medium- substitution at vinylic and allylic carbons - Aromatic nucleophilic substitutions –mechanisms –  $S_N^Ar$ ,  $S_N^1$ , -Benzyne –reactivity-effect of substrate, leaving group and attacking nucleophile

**Unit – II - Electrophilic substitution reaction**

Aliphatic electrophilic substitution –Arenium ion mechanism –Orientation and reactivity in monosubstituted benzene rings – benzene rings with more than one substituent –effect of leaving group –o/p ratio - Addition to C-C –multiple bonds – mechanisms-eletrophilic, nucleophilic, free radical – orientation and reactivity – addition of conjugated systems.

Elimination – mechanisms of  $\beta$  elimination –( $E_2, E_1, E_{1CB}$ ) - orientation of double bonds-reactivity- effect of substrate, attacking base, leaving group and medium.

### Unit - III - Stereochemistry

Stereoisomerism- definitions and classification – molecular representation and inter conversion - introduction to molecular symmetry and point groups with examples- Conformation analysis-cyclic system-cyclohexane –conformation and reactivity with examples from molecular rearrangements - Stereoselectivity- classification, terminology, principle of stereoselectivity, example of diastereoselectivity and enantioselectivity including few examples from pericyclic reactions- circular dichroism-ORD-cotton effect-application of ORD.

### Unit -IV - Reagents in organic synthesis

Use of the following reagents in organic synthesis and functional group transformations-complex metal hydrides, Hilman,s reagent, lithium dimethyl cuprate, lithium diisopropyl amide (LDA), dicyclohexyl carbodimide,1,3-dithiane, woodward and provost hydroxylation,DDQ, selenium dioxide, crown ethers and peterson's synthesis,wilkinson's catalyst, Baker yeast

### Unit – V Heterocyclics and supramolecules

Hetero cyclics – Nomenclature – compounds containing two hetero atoms – azoles- chemistry of pyrazole, imidazole, oxazole, isoxazole, thiazole and isothiazole-diazines-pyrimidines - Supramolecular chemistry – preparation and structure of catananes and rotaxanes - molecular recognition-synthetic applications of calixarenes and cyclodextrines-organic reactions on solid supports zeolite, clay,alumina and silica

#### Text Books:

1. Peter Sykes, “Advanced organic chemistry, Reaction mechanisms”, Longman and scientific technical, New York, 1985 (for 1-3 units)
2. R.T Morrison and R.N.Boyd, “Organic Chemistry”, PrenticeHall-Inc., New Jersey, 1992 (for 4 – 5 units)

#### Reference Books:

1. Jerry March “Advaned Organic Chemistry”, Wiley Eastern Limited , Fourth edition,, New Delhi,1999.
2. Rai K.Bansal ,”Organic reaction mechanism” Tata McGraw Hill,NewDelhi,1990.
3. F.A.Cary,”Organic chemistry” second edition,McGrawHill,Inc.,1992.
4. P.S.Kalsi,”Stererochemistry “,Wiley Eastern Limited ,New Delhi,1990.
5. R.O.C.Norman,”Principles of organic synthesis” second edition, Chapman and Hall,London,Newyork,1978.

6. V.K.Ahluwalia and Ram Agarwal ,”Organic synthesis”, Narosa Publishing House,NewDelhi.
7. I.L.Finar,” Organic chemistry” Vol I,ELBS,fifth edition,1989.
8. R.K.Bansal,”Heterocyclic Chemistry”, Wiley eastern ,1990.

## **09CH365 - RESEARCH METHODOLOGY IN CHEMISTRY**

**Credit: 4:0:0**

### **Objectives:**

1. Deals about the introduction to research, literature review
2. Detailed discussion about research designs and data analysis and various problem solving methods
3. Presents a clear way how to write research papers and presentation methodology
4. Deals about error analysis in chemical measurements and results

### **Unit - I Introduction to research**

Introduction – scientific investigation – research process – broad problem area - preliminary problem identification and analysis – design of research sources - completion of research methodology.

### **Unit – II Literature review**

Introduction – aim – content – surveying – synthesizing – critical analysis – reading materials – reviewing – rethinking – selection of sources – critical evaluation – interpretation – academic language – advantages.

### **Unit – III Research design and data analysis**

Research design - qualitative and quantitative research – sources of data – data collection procedures – measurement strategies – content analysis – literature surveys – information databases – statistical techniques – evaluation – development of a research program.

**Problem solving methods:** Methods for problem solving – analytical methods – numerical methods – computer simulation – experimental methods – development of a research question – sharpening objectives – identifying a problem – critical review of published literature – time management and management by crisis – budget management.

### **Unit – IV Presentation and research paper writing**

Technical paper writing – MS office and Typing exercises – data base – computer graphics – charts, diagrams – internet surfing and literature search – introduction to power point – power point presentation – multiple regression exercise – analyze data – excel worksheets – chart preparation.

**Unit – V Error analysis in chemical measurements and results**

Various types of errors – precision and accuracy – significant figures – various statistical tests on the accuracy of results – positive and negative deviation from accurate results – the binomial distribution – the Gaussian distribution – the normal distribution of random errors – mean value – variance and standard deviation – reliability interval – deviations from the Gaussian law of error distribution – student's *t* – distributions and 't' tests – comparison of the mean with the expected value – comparison of the results of two different methods – comparison of the precision of two methods by F-test – Gross errors and elimination of outlying results – graphical methods – linear regression – regression line – standard deviation – correlation coefficient – multiple linear regression (one variable with two other variables)

**Text Books:**

1. R. Burns, "Introduction to Research Methods", Addison Wesley Longman, Third Edition, 1997
1. C. R. Kothari, "Research Methodology: Methods and Techniques", New- Age International, 2008
2. S.Usharani, "Analytical Chemistry", first edition, Mcmillan, India Ltd, 2000.

**Reference Books:**

1. Nicholus Walliman "Your research project"- SAGE publication.2001.
2. K. Eckschlager, "Errors, Measurement and Results in Chemical Analysis", Van Nostrand Reinhold Company, London, 1991, Chapters 1, 4, 5
3. K. V. Raman, "Computer in Chemistry", Tata McGraw Hill, New Delhi, 1993

# **DEPARTMENT OF CHEMISTRY**

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Karunya University

## REVISED AND NEW SUBJECTS

| Code    | Subject Name                      | Credit |
|---------|-----------------------------------|--------|
| 10CH301 | Physical Chemistry - I            | 4:0:0  |
| 10CH302 | Organic Chemistry - I             | 4:0:0  |
| 10CH303 | Analytical Chemistry - I          | 4:0:0  |
| 10CH304 | Physical Chemistry - II           | 4:0:0  |
| 10CH305 | Organic Chemistry - II            | 4:0:0  |
| 10CH306 | Analytical Chemistry – II         | 4:0:0  |
| 10CH307 | Physical Chemistry - III          | 4:0:0  |
| 10CH308 | Organic Chemistry - III           | 4:0:0  |
| 10CH309 | Polymer Chemistry                 | 4:0:0  |
| 10CH310 | Advanced Pharmaceutical Chemistry | 4:0:0  |
| 10CH311 | Industrial Electrochemistry       | 4:0:0  |

### 10CH301 Physical Chemistry – I

**Credits 4:0:0**

#### Course Objectives:

- To know about Chemical thermodynamics & statistical thermodynamics
- To know about phase rule for one component, two component and three component systems
- To know about surface chemistry

#### Outcome

- Students acquire a good understanding of the basic principles of chemical and statistical thermodynamics, application of phase rule to different chemical systems and surface chemistry principles

#### Unit I : Chemical thermodynamics

First law of thermodynamics – Limitation of first law of thermodynamics - Second law of thermodynamics – Third law of thermodynamics – Entropy – Entropy change in phase transformations – Entropy changes of an ideal gas in different processes – Entropy at absolute zero – Determination of absolute entropies of solids, liquids and gases – Trouton's rule - Partial molar properties – Chemical potential – Gibbs – Duhem equation – Variation of chemical potential with temperature and pressure – Activity – Activity coefficient – Ideal solution – Real solution – Fugacity – Determination of a fugacity of a gas.

#### Unit II : Surface chemistry

Adsorption of gases by solids – Langmuir, Freundlich and B-E-T isotherms – applicability to heterogeneous catalysis – determination of surface area of adsorbents – Electrokinetic phenomena – Donnan membrane equilibrium – emulsions

### **Unit III : Phase rule**

Gibbs phase rule and phase equilibria – Degree of freedom – One component system – Water system – Sulphur system – Carbon-di-oxide system – Carbon system – Helium System – Two components system – Reduced phase rule – Lead – silver system – Pattinson's process – Ferric chloride – water system – Potassium iodide–water system – Sodium chloride–water system – Sodium–potassium system – Zinc-magnesium alloy system – Copper-nickel alloy system – sodium-sulphate system – Iron-carbon alloy system – Three component system – Brief description about two salts and water system – Allotropy – Heat treatment.

### **Unit IV : Statistical thermodynamics – I**

Concepts of probability and Maxwell Boltzmann distribution – Basic derivation – prove that  $\beta = 1/KT$  – Relationship between entropy and thermodynamic probability systems with degeneracy – Definitions of partition function – applications – derivation of thermodynamic functions from partition function – entropy for monoatomic gases – Sackur – Tetrode equation – The Bose – Einstein's system – Basic derivation – Fermi – Dirac system – Basic derivation – negative Kelvin temperature

### **Unit V : Statistical thermodynamics – II**

Heat capacity of solids – Debye and Einstein models – Thermodynamics functions of ideal gases, translational, vibrational and rotational contributions at different levels of approximation

Irreversible thermodynamics – the steady – coupled flows – application – over potential – decomposition potential – electrical double layer – structure of electrical double layer – capacity – steaming potential – electro dialysis – the Dorn effect

#### **Text books:**

1. P.W. Atkins, "Physical Chemistry", 8<sup>th</sup> edition, Oxford University Press, 2006
2. B.R., Puri, L.R. Sharma and Madan S. Pathania, "Principles of Physical Chemistry", Shoban Lal Nagin Chand & Co., Jalandhar, 2000
3. Kundu and S.K. Jain, "Physical Chemistry" S. Chand & Company Ltd., New Delhi, 1984
4. Duncan Shaw, "Introduction to colloid and surface chemistry", Elsevier, 1992

#### **Reference Books:**

1. J. C. Kuriacose and J.Rajaram, "Thermodynamics", Shoban Lal Nagin Chand & Co., Jalandhur, 1996
2. G.W. Castellan, "Physical Chemistry", Narosa publishing house, Chennai, 1989
3. H. Snehe, "Comprehensive Physical Chemistry", Prgati Prakashan, Meerut, 1987
4. S. Glasstone and D.Lewis, "Elements of Physical Chemistry", 2<sup>nd</sup> Ed., 1982
5. N.D. Smith, "Elementary Statistical Thermodynamics", Plenum Press, New York, 1982
6. B.C. McClelland, "Statistical Thermodynamics", Chapman and Hall, London, 1973
7. M. C. Gupta, "Statistical Thermodynamics", Wiley Eastern Limited, 1993
8. L.K. Nash, "Elements of classical the statistical thermodynamics", Addison-Wesley 1970

9. S Glasstone, "Thermodynamics for Chemists", Affiliated West Wes Press, New Delhi, 1965
10. Gabor A. Somorjai, "Surface Chemistry and Catalysis", Wiley, New York, 1994

## 10CH302 ORGANIC CHEMISTRY – I

**Credits 4:0:0**

### **Course objectives:**

To enable the student to understand (a) The stereochemistry of organic reactions (b) The detailed mechanism of all kind of organic reactions.

### **Outcome:**

Students can carryout organic reactions with proper understanding and knowledge of mechanism and orientation changes.

### **Unit I: Stereochemistry – I**

Stereoisomerism – definitions and classification – molecular representation and inter conversion – Classification of stereo isomers – Stereoisomerism and center of chirality – molecules with a single stereogenic center – Projection structure of stereoisomers – Fischer – DL, RS and EZ notations - configurational nomenclature – molecules with two or more chiral centers – Stereoisomerism in cyclic compounds – axial chirality, planar chirality and helicity – molecules with axial chirality

### **Unit II: Stereochemistry – II**

Difference between conformation and configuration – conformation of ethane, substituted ethanes – conformation of cyclohexanes, mono, and disubstituted cyclohexanes – saw-horse, staggered, skew, gauche forms – explanation and conversion of one representation to another – fused ring systems – decalins – biphenyls - Stereoisomerism in Allenes  
Dynamic stereochemistry: Stereoselectivity and stereospecificity – Curtin-Hammett principle – enantioselective, diastereoselective synthesis – enzymatic and kinetic methods – Sharpless asymmetric epoxidation – conformation and reactivity in acyclic compounds and cyclohexanes

### **Unit III: Reaction Mechanism – I**

Effect of structure and reactivity – Resonance and field effects – Steric effects – Quantitative treatments of the effect of structure and reactivity – LFER – Hammett and Taft equation - Importance of  $\sigma$  and  $\rho$  values in aromatic electrophilic substitutions – Labelling and kinetic isotopic effects.

Aromaticity – Huckel's rule – Aromatic systems with electron numbers other than six – annulenes and hetero annulenes – Chemistry of fullerenes.

### **Unit IV: Reaction Mechanism – II**

Aliphatic nucleophilic substitution – mechanisms –  $S_N^2$ ,  $S_N^1$ , mixed  $S_N^1$  and  $S_N^2$ ,  $S_N^i$ , SET, neighbouring group mechanism – Reactivity – effect of substrate, attacking nucleophile, leaving group and reaction medium – Substitution at vinylic and allylic carbons.  
Aromatic nucleophilic substitutions – mechanism -  $S_N^{Ar}$  -  $S_N^1$  – Benzynes – reactivity – effect of substrate, leaving group and attacking nucleophile.

### Unit V: Reaction Mechanism – III

Aromatic electrophilic substitution – Arenium ion mechanism – Orientation and reactivity in monosubstituted benzene rings – benzene rings with more than one substituent - effect of leaving group – o/p ratio.

Addition to C-C-multiple bonds – mechanisms – electrophilic, nucleophilic, free radical – orientation and reactivity – addition of conjugated systems

Elimination – mechanisms of  $\beta$  elimination – ( $E_2$ ,  $E_1$ ,  $E_{1CB}$ ) –  $E_1$  –  $E_2$  –  $E_{1CB}$  spectrum, orientation of double bonds – reactivity – effect of substrate, attacking base, leaving group and medium.

#### Text Books:

1. Jerry March, “Advanced Organic Chemistry”, Wiley Eastern Limited, Fourth edition, New Delhi, 2008
2. Morrison and Boyd, “Organic Chemistry”, 3<sup>rd</sup> edition, United states of America, 1992
3. B. S. Bahl and Arun Bahl, “Text book of Organic Chemistry”, New Delhi, S. Chand & company Ltd., 2009
4. Peter Skyes, “A Guidebook to Mechanism in Organic Chemistry”. Longman Press, London and New York, 2006
5. Ernest. L. Eliel, “Stereochemistry of carbon compounds”, 22<sup>nd</sup> reprint, Tata-McGraw Hill, New Delhi, 2009

#### Reference Books:

1. D. Nasipuri, “Stereochemistry of organic compounds – Principles and applications” 2<sup>nd</sup> edition, New Age international, 2002
2. T.W.G. Solomons, “Organic Chemistry”, Vol.2, ELBS, 1989
3. Indian Journal of Chemistry (A and B), special issues on Fullerenes, Vol. 31 A, A & B, No. 5, March 1992
4. Rai K. Bansal, “Organic reaction mechanism”, Tata McGraw Hill, New Delhi, 1990
5. F.A. Cary, “Organic Chemistry”, Second edition, McGraw Hill, Inc., 1992
6. P.S. Kalsi, “Stereochemistry”, Wiley Eastern Limited, New Delhi, 1990
7. V.M. Potapov, “Stereochemistry” Mir Publisheres, Moscow, 1979
8. R. Curl, Accounts of Chemical Research, “Special issue on Buckminster Fullerenes”, Vol. 25, No. 3, March 1992, pages 98 - 105
9. I.L. Finar, “Organic Chemistry, Volume 1: The Fundamental Principles”, London Longmans, 1963

### 10CH303 Analytical Chemistry – I

Credits 4:0:0

### **Course Objectives:**

- The student will learn how to analyze data and calculate error
- The principles of titrations and estimations the student does in the lab will be taught
- The methods of separation of chemical compounds will be understood by him
- Analysis of samples with spectral techniques will be taught to the students

### **Outcome:**

- The student will get theoretical background on the experiments he does, analyzes and the calculation procedures for the parameters he/she wants to derive at.

### **Unit I: Introduction to analytical methods**

Errors - accuracy and precision – standard deviation - student's confidence interval of the mean – significant figures and computation rules – correlation coefficient

Gravimetric analysis: solubility product – common ion effect – co-precipitation – purity of precipitates – conditions of precipitation – Complexometry: EDTA titrations – mask and demasking agents – determination of Zn, Mg, Mn, and Ni by EDTA titration

### **Unit 2: Chromatography**

Column chromatography: principles and applications – ion exchange chromatography – elutropic series – gas chromatography: instrumentation, principle and applications – High Performance Liquid Chromatography: instrumentation, principles and applications – Ion chromatography – principles – applications towards separation of cations (Zn and Mg, Zn and Cd) – applications towards separation of anions (Chloride and bromide, chloride and nitrate) – Gel permeation chromatography – Solid-liquid chromatography

### **Unit III: Diffraction methods and crystallography**

Seven crystal systems - isomorphism and polymorphism, laws of crystallography, lattice types, X-ray diffraction, Bragg's equation, Bragg method, structure of simple lattice and X-ray intensities, structure factor and its relation to intensity and electron density – Neutron diffraction – principle and applications

### **Unit IV: Vibrational spectroscopy**

General introduction to electromagnetic spectrum – IR spectroscopy: instrumentation - the vibrating diatomic molecule – factors influencing vibrational frequencies - vibrational transitions - selection rule – anharmonic oscillator – vibrations of polyatomic molecules – fundamental bands and overtones – identification of functional groups – finger print region – application to organic and inorganic compounds – Simple problems in functional group identification using IR spectrum

### **Unit V: Ultraviolet and visible spectroscopy**

Electronic spectra of diatomic molecules - instrumentation of uv spectroscopy – physical principles – laws of absorption – absorption transitions – chromophores and auxochromes – effects of conjugation – Woodward-Fieser rules for  $\alpha,\beta$ -unsaturated carbonyl compounds and dienes – aromatic systems with extended conjugation – Simple problems using Woodward-Fieser rule - Principles of optical rotatory dispersion (ORD) and circular dichroism (CD) –

Cotton effect – octant rule – axial haloketone rule – applications of ORD and CD in organic and bio-molecules

**Text Books:**

1. Y.R. Sharma, Elements of Organic Spectroscopy, S. Chand & Company Ltd., New Delhi, 2004
2. C. N. Banwell & E. M. McCash, Fundamentals of Molecular Spectroscopy, 4<sup>th</sup> Edition, McGraw-Hill, New Delhi, 2004
3. Jag Mohan, Organic Spectroscopy Principles and Applications, Narosa Publishing House, New Delhi, 2001
4. G.H. Geffery, J. Bassett, J. Mendham, R.C. Denney, Ed. V, Vogel's textbook of quantitative chemical analysis, Longman Group UK Ltd., 1989

**Reference Books:**

1. D.N. Satya Narayana, Vibrational Spectroscopy Theory and Applications, New Age International Publishers, New Delhi, 2004
2. K.L. Kapoor, Text Book Physical Chemistry, Vol. I & II, Mac Millan India Ltd., New Delhi, 1994
3. A.G. Whittakar, Physical Chemistry, Mount & Heal Viva Books Pvt. Ltd., New Delhi, 2001
4. C. Kittel, Introduction to solid state physics, , John Wiley & sons, Ed. 6, 1953
5. J. D. Hoffman, Numerical methods for engineers and scientists, Marcel Dekker Inc., 2001
6. H. willard, L.Meritt, J.A. Dean and F.A. settle, Instrumental methods of chemical analysis by, Sixth edition CBS, 1986
7. Galen W. Ewing, Instrumental Methods of Chemical Analysis, Mc Graw Hill Int. Editions, 3<sup>rd</sup> Edition, Singapore, 1988

**10CH304 PHYSICAL CHEMISTRY – II**

**Credits 4:0:0**

**Course Objectives:**

- To know about chemical kinetics, mechanism of gas phase reactions, catalysis & quantum mechanics

**Outcome**

- Students acquire a good knowledge on the chemical kinetics, mechanism of gas phase reactions, catalysis and quantum chemistry of atoms and molecules.

**Unit I : Chemical kinetics**

Chemical kinetics – Basic concepts – rate law – rate equation – Kinetics of zero, first, second and third order reactions – Kinetics – composite reactions (complex reaction) – Opposing (reversible) reactions – Consecutive reactions – Chain reactions – Stationary chain reaction – Non-stationary chain reaction – Collision theory of bimolecular and unimolecular reactions – Arrhenius theory of reaction rates – Theory of absolute reaction rates – Thermodynamic

treatment of reaction rate – Kinetics of fast reactions – Hammett relationship - ionic reactions in solution – effect of ionic strength.

### **Unit II : Mechanism of gas phase reactions**

Chemiluminescence – reactions in molecular beam – Lindemann's theory – Hinshelwood, Kassel and Slater's treatments – Reaction rates in solution - Effect of dielectric constant and ionic strength – Kinetic isotope effect – Linear free energy relationships – Taft equation – Yukawa-Tsuno equation – Luminescence and energy transformations – Study of kinetics of stopped flow techniques – flash photolysis – shock tubes.

### **Unit III : Catalysis**

Acid – Base catalysis – general scheme – Arrhenius complex – Vant Hoff's complex – specific and general catalysis – catalytic constants – Bronsted relationship – Hammett acidity functions – mechanism of acid-base catalysed reaction – Catalysis by metal salts (transition metal complex) – enzyme catalysis – theory and applications - Mechanism of heterogeneous catalysis - Langmuir- Hinshelwood mechanism and Langmuir Reidel mechanism - Examples of heterogeneous catalytic reactions - hydrogenation of ethylene , synthesis of ammonia, oxidation of SO<sub>2</sub> and Fischer- Tropsch method for the synthesis of methanol - Gibbs adsorption equation

### **Unit IV : Introduction to quantum mechanics**

The failures of classical mechanism – heat capacities – black body radiation – The photo electric effect – The Compton effect – The diffraction of electrons – Atomic and molecular spectra, wave particles duality – Uncertainty principle, operators and commutation relations – Postulates of quantum mechanics – Scrodinger equation, Free particle, particle in one dimensional box, three dimensional box – Harmonic oscillator – Rigid rotor – The Schrodinger equation for hydrogen atom – Angular momentum – Spin, coupling of angular momentum – Spin-orbit coupling.

### **Unit V : Quantum chemistry of atoms and molecules**

Variation and perturbation theory – Application of perturbation / variation theorems to ground state of helium atom – Antisymmetry and Pauli's exclusion principle – Aufbau principle – Slater detrimental wave functions – Term symbols and spectroscopic states – Born Oppenheimer approximation – LCAO, MO and VB treatments of hydrogen molecule – MO treatment of large molecules with symmetry – Hybridization – Huckel theory of linear conjugated systems – Cyclic systems – Wood- ward Hoffman rules.

### **Text Books:**

1. A.W. Adamson, "Physical Chemistry of Surfaces", 5<sup>th</sup> edition, Wiley, 1990
2. K.J. Laidler, "Chemical Kinetics", Harper and Row, New York, 3<sup>rd</sup> Edition, 2008
3. Donald A McQuarrie, "Quantum Chemistry", University Science Books, Mill Valley, California, 1983.
4. AK Chandra, "Introduction to Quantum Chemistry", Tata McGraw Hill, New Delhi, 2001
5. John C. Schug, "Introductory Quantum Chemistry", Holt, R & W Publisher, 1972

**Reference Books:**

1. J. Rajaram and J.C. Kuriakose, "Kinetics and mechanism of chemical transformation", McMillan India Ltd., New Delhi, 1993
2. C. Kalidas, "Chemical Kinetic Methods: Principles of Relaxations Techniques and application", New Age International (P) Ltd, Chennai, 1996
3. P.W. Atkins, "Molecular Quantum Mechanics", 2<sup>nd</sup> edition, Oxford University Press, 1983
4. I.N. Levine, "Quantum Chemistry", 4<sup>th</sup> edition, Prentice Hall India, 1994
5. M.W. Hanna, "Quantum Mechanics in Chemistry", 3<sup>rd</sup> edition, Addition Wisley, London, 1981

**10CH305 ORGANIC CHEMISTRY - II****Credits 4:0:0****Course Objectives:**

- To enable the student to understand
  - (a) The principles of organic synthesis
  - (b) Reagents used in organic synthesis
  - (c) Photochemical, pericyclic, and different Molecular rearrangements

**Outcome:**

- Students can make use of different reagents in organic synthesis and they can do it in different pathways.

**Unit I: Principles of organic synthesis**

The synthesis process – preliminary planning, molecular characteristics, functional group transformation – retrosynthetic analysis – order of events – one group – C – X disconnection – Chemo selectivity two group C- X disconnection – chemo selectivity two group C-X disconnection – reversal of polarity – cyclisation reactions – protecting groups – one group disconnection C-C, alcohols, C=O, stereoselectivity – regioselectivity

**Unit II: Organic name reactions and reagents used in organic synthesis**

Organic name reactions: Favorskii reaction - Michael addition - Mannich reaction - Stork - Enamine reaction –MPV reduction, oppenauer oxidation, Sharpless asymmetric epoxidation - Ene reaction - Barton reaction - Chichibabin reaction - Fischer – indole synthesis. Use of the following reagents in organic synthesis and functional group transformations - Complex metal hybrids - Gilman's reagent - lithium dimethylcuprate - lithium disopropylamide (LDA)- osmium tetroxide – DDQ - selenium dioxide - Merrified resin

**Unit III: Pericyclic reaction**

Definition – types – Woodward-Hofmann rules, orbital correlation diagrams, FMO treatment, PMO method, electrocyclic conversion of 1,3-dienes and 1,3,5-trienes – cycloadditions – 2+2 addition, Diels-Alder reaction, sigmatropic reactions – cope and claisen rearrangement.

#### **Unit IV: Organic Photo Chemistry**

Introduction – Interaction of electromagnetic radiation with matter – electronic excitations – excited states – transfer of excitation energy – sensitization and quenching – photochemical eliminations, Norrish type I and II reactions, Paterno-Buchi reaction, oxidations – reductions, cis-trans isomerisation, rearrangements (di-pi methane or Zimmerman rearrangement).

#### **Unit – V: Molecular rearrangements**

Mechanism of the following rearrangement reactions – Pinacol-Pinacolone rearrangement – Wagner-Meerwein rearrangement– Hofmann rearrangement– Beckmann rearrangement – Curtius rearrangement – Wolff rearrangement – Baeyer-Villiger reaction – Dakin reaction – Stevens rearrangement – Sommelet rearrangement – Wittig rearrangement – Benzidine rearrangement– Benzil-Benzilic acid rearrangement – Cope rearrangement – Dienone rearrangement

#### **Text Books:**

1. I.L. Finar, "Organic Chemistry" Vol.2, ELBS, 6<sup>th</sup> edition, Singapore, 2008.
2. Robert E. Ireland, "Organic synthesis", 2<sup>nd</sup> edition, Prentice-Hall of India Pvt. Ltd., New Delhi, 1988
3. V.K. Ahluwalia and Ram Aggarwal, "Organic Synthesis", Narosa Publishing House, New Delhi
4. G.R. Chatwal, "Organic photo chemistry" 1<sup>st</sup> edition, Himalaya Publishing House, Mumbai, 2008.
5. A. Hassner and C. Stumber, "Organic Synthesis based on name reactions", Pergamon, 2002
6. S.M.Mukherji and S.P.Singh, Reaction Mechanism in Organic Chemistry, 1<sup>st</sup> Edition, Macmillan, 1976
7. Jagadamba Singh, "Organic Synthesis", Prgati Prakashan,
8. Jerry March, "Advanced Organic Chemistry – Reactions, Mechanisms and structure, 4<sup>th</sup> edition, John Wiley & Sons, 2008.
9. Gurdeep R. Chatwal, "Reaction Mechanism and Reagents in Organic Chemistry", Himalaya Publishing House, New Delhi, 2007.

#### **Reference Books:**

1. R.O.C. Norman, "Principles of organic synthesis" 2<sup>nd</sup> edition, Chapman and Hall, London, New York, 1978
2. J.M. Coxon, B. Halton, "Organic photochemistry", Cambridge University Press, 2<sup>nd</sup> edition, 1987
3. Andre Loupy, "Solvent free reactions", Topics in current chemistry, Vol. 206, Page 155 –173
4. W. Carruthers, "Some modern methods of organic synthesis", Cambridge university press, 3<sup>rd</sup> edition, 1988
5. T.L. Gilchrist & R.C. Storr, "Organic reaction orbital symmetry", Cambridge university press, 1972

6. F.A. Carey and R.J. Sundberg, "Advanced Organic Chemistry Part – B: Reactions and Synthesis, Plenum Press, 2008

## 10CH306 ANALYTICAL CHEMISTRY – II

**Credits 4:0:0**

**Course Objectives:**

- The student will understand structure determination using spectral analysis
- The physical principles and their application in analytical methods will be taught to the students
- The student will understand the differences between absorption and emission spectroscopic techniques and their applications

**Outcome:**

- The student will become an expert in analyzing spectral data and structure elucidation

**Unit I: NMR spectroscopy and ESR spectroscopy**

Physical principle of NMR spectroscopy – instrumentation – proton NMR – Difference between continuous wave and FT NMR - chemical shift - factors affecting chemical shifts – chemical and magnetic equivalence – Mechanisms of nuclear relaxation – spin-spin coupling in AB, A<sub>2</sub>B<sub>2</sub>, and ABX systems – C-13 NMR - application of H-1 NMR and C-13 NMR to organic compounds – Decoupling – Off-resonance decoupling – Simple problems in structure determination using H-1 NMR

ESR Spectroscopy: principles, factors affecting intensity, position, and multiplet structure of spectra – hyperfine splitting – zero field splitting – Kramer's degeneracy – applications.

**Unit II: Thermal methods, photoelectron spectroscopy and Mössbauer spectroscopy**

Principles and instrumentation of thermo-gravimetric analysis (TGA) and differential thermal analysis (DTA) – complementary nature of TGA and DTA – differential scanning calorimeter (DSC) – isothermal titration calorimetry (ITC) – applications of thermal methods in the study of minerals, polymers, and biological molecules

Ultraviolet photoelectron spectroscopy (UPS) - X-ray photoelectron spectroscopy (XPS) – Electron spectroscopy for chemical analysis (ESCA) – principles and applications of the above methods - Mössbauer spectroscopy – principles – spectrometer – nuclear Zeeman splitting – isomer shift – quadrupolar interaction – hyperfine interactions – applications

**Unit III: Mass spectrometry**

Principle of mass spectrometry – mass spectrometers - determination of molecular formula – nitrogen rule – meta-stable ions and peaks – molecular ion peak – fragmentation processes – even and odd electron ions – retro-Diels-Alder rearrangement – McLafferty rearrangement – fragmentation associated with functional groups – aldehydes and ketones, aromatic compounds

**Unit IV: Electro-analytical techniques**

Electro-analytical techniques: Coulometry and amperometric titrations – principle and instrumentation – primary and secondary coulometric analysis – coulometry at controlled potential – coulometry at constant current – voltammetric techniques – polarography – DME – advantages of dropping mercury electrode – DC, TAST, normal pulse, differential pulse – cyclic voltammetry – principle, instrumentation, application

### **Unit V: Fluorescence Spectroscopy**

Principles of fluorescence - static and dynamic quenching of fluorescence – steady-state and time-resolved fluorescence - excited state intra-molecular proton transfer (ESIPT) – intramolecular charge transfer (ICT) – fluorescence resonance energy transfer (FRET) – fluorescence anisotropy - fluorescence correlation spectroscopy (FCS) – fluorescence confocal microscopy – principles and applications of the above methods

#### **Text Books:**

1. Gurdeep R. Chatwal & S. K. Anand, Spectroscopy, Himalaya Publishing House Mumbai, 2004
2. Gupta Kumar & Sharma, Elements of Spectroscopy, Pragati Prakasan, Meerut, 2001
3. P.S. Kalsi, Spectroscopy of Organic Compounds, 6th Edition, New Age International Publishers, New Delhi, 2004
4. V. Gopalan, P.S. Subramanian, K. Rangarajan, Elements of Analytical Chemistry, S. Chand and Sons, New Delhi, 2003

#### **Reference Books:**

1. B.P. Straughan & S. Walker, Spectroscopy, John Wiley and Sons, New York, 1976
2. Y.R. Sharma, Elements of Organic Spectroscopy, S. Chand & Company Ltd., New Delhi, 2004
3. C. N. Banwell & E. M. McCash, Fundamentals of Molecular Spectroscopy, 4<sup>th</sup> Edition, McGraw-Hill, New Delhi, 2004
4. Jag Mohan, Organic Spectroscopy Principles and Applications, Narosa Publishing House, New Delhi, 2001
5. R. M. Silverstein, C. Bassler, & F. X. Webster, Spectroscopy of Organic Compounds, 6<sup>th</sup> Edition, Wiley Publications, 1998
6. Galen W. Ewing, Instrumental Methods of Chemical Analysis, 3<sup>rd</sup> Edition, Mc Graw Hill Int. Editions, Singapore, 1988
7. Fluorescence spectroscopy, J.R. Lakowicz, Ed. II, Wiley-VCH publishers, 2004
8. H. Willard, L. Merrit, J.A. Dean and F.A. Settle, Instrumental methods of chemical analysis by, Sixth edition CBS, 1986

### **10CH307 PHYSICAL CHEMISTRY – III**

**Credits 4:0:0**

**Course Objectives:**

- To know about basics and applications of group theory
- To understand the fundamental and applied concepts of photo chemistry, electrochemistry and nanotechnology.

**Outcome:**

- Students acquire knowledge on the basics of group theory, applications of group theory, practical applications of photochemical reactions, electrochemistry principles and nanotechnology

**Unit I : Group Theory**

Molecular symmetry – symmetry elements and symmetry operations-successive operations, inverse operations - Cartesian coordinate system - relations among symmetry elements - Properties of a group – Abelian, non abelian and Isomorphic groups - Multiplication tables – classes, subgroups - Molecular point groups - Schoenflies symbols - Matrices of symmetry operations - Representations of a group-Reducible and irreducible, representations - Statement and proof of Great orthogonality theorem - Characters and construction of character table ( $C_{2v}$ ,  $C_{3v}$ ) – Explanation of a character table - Direct product groups

**Unit II : Applications of Group Theory**

Standard reduction formula relating reducible and irreducible representations -Symmetries of normal modes of vibration in non-linear molecules ( $H_2O$ ,  $NH_3$ ,  $BF_3$ ) - Selection rules for vibrational spectra – IR and Raman active fundamentals – Mutual exclusion rule - Symmetries of M.O and symmetry selection rule for electronic transition in ethylene and formaldehyde - Hybridization schemes for atoms in methane, ethylene and butadiene.

**Unit III : Photo Chemistry**

Absorption and emission of radiation – Theories – Spontaneous and induced emission – Maser and Laser – Franck Condon principle – Physical properties of electronic excited state – Emission – Resonance emission – Fluorescence – Phosphorescence – Jablonski diagram – Internal conversion (IC) – Intersystem crossing (ISC) – Delayed fluorescence: E-Type and P-Type – Excimer and Exciplex complex formation – Stern-Volmer equation and derivations – Photosensitization and Chemiluminescence – Experimental techniques – Chemical actinometry – Flash photolysis – Important photochemical reactions: Photoreduction – Photooxidation – Photosubstitution – Elementary ideas of photosynthesis and solar energy conversion.

**Unit IV : Introduction to Applied Electrochemistry**

Theories of electrical double layer (EDL) – EDL at the electrode – electrolyte interface-Helmholtz model of DL - Electrode kinetics – Butler Volmer equation–Derivation of the equations-Tafel equation and plots - Hydrogen overpotential – Mechanism of hydrogen evolution reactions – Theories of hydrogen overvoltage - Passivity (chemical and mechanical passivity) - Corrosion (definition, theory, methods of preventing corrosion) - Polarography – Dropping mercury electrode – half wave potential and applications – Introduction to Electrochemical energy conversions.

## Unit V : Nano Technology

Nanomaterials – Preparation: Plasma arcing - Chemical vapor deposition – Sol-gels – silica gels – Hydrolysis – Condensation and polymerization of monomers to form particles – Zirconia and yttrium gels – Aluminosilicate gels – Forming nanostructured surfaces using the sol – gel process – Trapping by sol –gels – Electrodeposition – Ball milling – Using natural nanoparticles – Applications of nano materials – Insulations materials - Machine tools – Phosphors – Batteries – High power magnets – Motor vehicles and aircraft – Medical applications

### Text Books:

1. K. Veera Reddy, “Symmetry and spectroscopy of molecules”, New Age International (P) Ltd., 2000
2. P.K. Bhattacharya, “Group Theory and its Chemical application”, Himalaya Publishing House, New Delhi, 1986
3. K.K. Rohatgi Mukherjee, “Fundamentals of photochemistry”, Wiley Eastern, New Delhi, 1986
4. Michael Wilson, Kamali Kannangara, Geoff Smith, Michelle Simmons and Burkhard Raguse, “Nanotechnology – Basic Science and Emergin Technologies”, Chapman & Hall (CRC), 2004
5. Samuel Glasstone, “An Introduction To Electrochemistry”, Maurice Press, 2007

### Reference Books:

1. F.A.Cotton, “Chemical application of group theory”, 2<sup>nd</sup> edition, Wiley-Interscience, New York, NY, 1971
2. K.V. Raman, “Group theory and its applications to chemistry”, Tata Mcgraw Hill, 2004
3. Alan Cox and T.J. Kemp, “Introductory photochemistry”, McGraw-Hill, 1971
4. John O'M. Bockris, Amulya K. N. Reddy, “Modern Electrochemistry Vol. I and II”, Plenum Publishing, 1970
5. Richard C. Alkire, Dieter M. Kolb, Jacek Lipkowski and Phil Ross, “Advances in Electrochemical Science and Engineering, Volume 9”, Wiley, 2006

## 10CH308 ORGANIC CHEMISTRY - III

**Credits 4:0:0**

**Course Objectives:** To enable the student to understand (a) Heterocyclic and supramolecular reactions (b) Natural products and its medicinal applications.

**Outcome:** Students will be aware of natural products and its medicinal use; they will get an outlook about chemical modification of natural products for its further applications.

### Unit I: Hetero cyclics and supramolecules

Heterocyclics – Nomenclature – compounds containing two hetero atoms – azoles – chemistry of pyrazole, imidazole, oxazole and thiazole– diazines – pyrimidines. Supra

molecular chemistry – preparation and structure of catenanes and rotaxanes – molecular recognition – synthetic applications of calixarenes and cyclodextrines.

### **Unit – II: Chemistry of Alkaloids and Terpenoids**

General methods of structure elucidation of alkaloids – structure, synthesis and stereochemistry of the following alkaloids – Quinine, Morphine, cocaine and reserpine  
Terpenoids - Classification - Structure, Stereochemistry and synthesis of camphor, Zingiberene, and abietic acid.

### **Unit – III: Natural Products– I**

Vitamins – introduction to vitamins A, B, C, D and E- synthesis of retinol and L-Ascorbic acid- Antibiotics and antibacterials - Antibiotic  $\beta$ -Lactam type - Penicillins - Antitubercular - Streptomycin - Broad spectrum antibiotics - Tetracyclines - Anticancer - Dactinomycin (Actinomycin D) - Antibacterial – Ciprofloxacin, Norfloxacin

### **Unit – IV: Natural Products – II**

Steroids – Introduction, Constitutional study of cholesterol, stereochemistry of steroids. Steroid hormones – Structural elucidation of progesterone, androsterone.

### **Unit – V: Anthocyanidins and Pigments**

Introduction – structure of anthocyanidins – general methods of synthesizing anthocyanidins - Cyanidin Chloride – Flavones – Flavonols - Iso flavones – Tannins.

### **Text Books:**

1. I.L.Finar, Organic Chemistry, Vol.2 – ELBS 6<sup>th</sup> Edition, 2008.
2. O. P.Agarwal, Chemistry of natural products, Vol.1, Goel publishing house, 36<sup>th</sup> edition, 2009.
3. A. Kar, “Medicinal Chemistry”, Wiley Eastern Ltd., New Delhi, 1993
4. W. O. Foye, “Principles of Medicinal Chemistry”, 3<sup>rd</sup> Edition, Lea & Febiger, Varghese Publishing House, Bombay, 1989
5. G. Schill, “Catenanes, Rotaxanes, and Knots”, Academic Press, New York, 1971
6. Morrison and Boyd, “Organic Chemistry”, Paramount Communications, 2007

### **Reference Books:**

1. Francis A. Carey, “Organic Chemistry”, 5th edition, Tata McGraw Hill, New Delhi, 2003.
2. Graham Solomns T.W, “Organic Chemistry”, Vol.I & II, 5th Edn, John Wiley & Sons, New York, 1992.
3. O.P.Agarwal, “Organic Chemistry Reactions and Reagents”.
4. Morrison and Boyd, “Organic Chemistry”, Paramount Communications, 2007
5. R.K. Bansal, “Heterocyclic Chemistry”, Wiley Eastern, 1990

## **10CH309 POLYMER CHEMISTRY**

**Credits 4:0:0**

## Course objectives

- To acquire complete knowledge about polymers

## Outcome

- Students would be able to understand the basic concepts of polymers, their properties, various fabrication techniques and finally new advanced materials like polymer nanocomposites

### Unit I. Basic concepts of polymers

Basic concepts of polymers – classification of polymers – ladder, star comb polymers tacticity – interpenetrating networks – structure property relationships – naturally occurring polymers – polysaccharides – cellulose and proteins – polymerization reactions – classifications – polymer resins – polymer solutions – reaction of polymers – introduction of new groups – cross linking, isomerisation, cyclisation and degradation reactions – Biopolymers – introduction and types

### Unit II. Principles of polymerization

Principles and mechanisms of polymerization – addition, step growth polymerization and coordination (i.e., Ziegler-Natta) – reactivity of functional groups – Carothers equation – kinetics – characteristics of step growth polymerization – examples – mechanisms, choice of monomers, effect of inhibitors or retarders, – co-polymerization – monomer reactivity – ratio – composition, types, the Q-e scheme.

### Unit III. Polymer properties

Molecular weight determination methods – Polymer stereochemistry – amorphous, crystalline and crystallites – viscous flow – viscosity – thermal behavior of polymers –  $T_g$ ,  $T_m$  and their relationships – elastic effect of polymers

### Unit IV. Polymerization processes and fabrication of plastics

Polymerization processes – bulk, solution, emulsion and suspension – industrially important polymers and their polymerization processes – polythene – poly styrene – nylon 6,6 – PET – natural rubber – Compounding of plastics – additives added and their significance – Moulding processes – injection, compression, blow moulding

### Unit V. Polymer nano-composites

Introduction to – conducting polymers and composites, applications in sensors, batteries – conventional composites – filler-matrix interaction, continuous (or long) and short fibre reinforced composites, laminates – Introduction to polymer nano-composites – clay, CNT, particle filled – advantages and limitations of nano fillers – surface treatment on nano-fillers – applications of polymer nano-composites – packaging, automotive, mechanical components.

## Text books:

1. A. Rudin, “The elements of polymer science and engineering”, Academic press, New York, 1982
2. V.R. Gowariker, “Polymer Science”, 5<sup>th</sup> edition, Wiley Eastern Ltd., 1992

3. G.S. Misra, "Introductory polymer chemistry", New Age International Pvt. Ltd., 1996
4. Anil Kumar and S.K. Gupta, "Fundamentals of polymer science and engineering" Tata McGraw Hill Publication Ltd., New Delhi, 1978
5. F W Billmeyer, Jr, "Textbook of Polymer Science" III edition, Wiley India 1984

**Reference books:**

1. David Sobolev, "A first course in polymer chemistry", MIR publishers, Moscow, 1971
2. R.J. Young, "Introduction to polymers" Chapman and Hall Ltd., London, 1981
3. D.H. Morton and Jones, "Polymer processing" Chapman and Hall, London, 1989
4. J.A. Brydson, "Plastic materials" 4<sup>th</sup> edition, Butterworth –Heinmann Ltd., London, 1995
5. J.A. Biesenberger and H. Sebastian, "Principles of polymerization engineering" , Wiley Interscience publications, New York, 1988
6. Stephen and Rosen, "Fundamental principles of polymeric materials" 2<sup>nd</sup> edition, John-Wiley and Sons Inc., New York, 1993
7. R B Seymour, "Introduction to Polymer Chemistry", Tata Mc GrawHill, New York, 1971
8. M Alexandre and P Dubois, Mater Sci Eng R Rep 28 (2000) 1

## 10CH310 ADVANCED PHARMACEUTICAL CHEMISTRY

**Credits 4:0:0**

**Course objective:**

To equip the students with a thorough understanding of different aspects of pharmaceutical chemistry

**Outcome:**

After finishing this course, the student will be able to understand and apply the design and synthetic approaches used in pharmaceutical chemistry.

**Unit I. Introduction to drug design**

Introduction to drug design, physical and chemical factors associated with biological activities, mechanism of drug action, drug delivery systems, classification of drugs based on structure or pharmacological basis with examples – mechanism of chemotherapeutic action – drug absorption across biological membrane – metabolism of drugs, Quantitative structure activity relationship - Molecular modeling – drug delivery, docking – structure based drug design – ligand based drug design – chirality in drug design

**Unit II. Drug discovery at the enzyme level**

Drug discovery at the enzyme level – chemical models and mimics for enzymes – receptor peptides, carbohydrates and other bioactive molecules – enzyme inhibitors – design and

synthesis – DNA – protein – interaction and DNA – drug interaction - enzymes in organic synthesis and combinatorial chemistry

### **Unit III. Drug action and drugs**

Drug action – Ideal requirement of a drug – sources of drug plant and animal origin synthetic and semisynthetic drug – terminology and short description of terms – Pharmacology, molecular pharmacology, pharmacognosy, pharmaco-kinetics, pharmacodynamics..

Analgesics – narcotic analgesics – morphine, analogues and modifications – codeine – synthetic narcotic antagonists – pethidines and methadones – narcotic analgesics – nalorphine – antipyretic analgesics – pyrazole – salicylic acid – para aminophenol derivatives – aspirin and salol.

### **Unit IV: Drugs acting on the Central Nervous System**

General Anesthetics(Cyclopropane, Fluoroxene, Halothane, Methoxyflurane, Trichloroethylene, Nitrous Oxide, Chloroform, Thiopental Sodium, ), Local Anesthetics(Ethyl-*p*-amino benzoate ; Butamben ; Orthocaine ; Procaine Hydrochloride, Tetracaine Hydrochloride ; Butacaine Sulfate Cyclomethycaine Sulphate), Hypnotics and Sedatives (Phenobarbitone, pentobarbitone, Chlordiazepoxide, diazepam, oxazepam), antiparkinsonism drugs(Biperiden Hydrochloride, dopamine), CNS stimulants (Amphetamine, Xanthine Derivatives).

### **Unit V: Varied class of drugs**

Structure of selected drugs, mode of action, uses, structure activity relationship (including physicochemical aspects) of the following classes of drugs (Biochemical approaches in drug designing wherever applicable should be discussed):

- i) Antimycobacterial Drugs- Pyrazinamide, isoniazid (INH) and rifampin (RIF), Fluoroquinolones, Ofloxacin, Ciprofloxacin Hydrochloride, Aminoglycosides
- ii) Antineoplastics agents- Alkylating Agents, Antibiotics, Antimetabolites.
- iii) Anti-viral including anti-HIV agents- Idoxuridine, Acyclovir, Vidarabine, Methisazone

#### **Text books:**

1. Ashutosh Kar, “Medicinal Chemistry” New Age Publishers, Fourth edition, 2007.

#### **Reference books:**

1. G.L. Patrick, “Introduction to medicinal chemistry”, Oxford University Press, 1995
2. F.S.K. Barar, “Essentials of Pharmacotherapeutics”, S. chand & Co., 1989
3. G.R. Marshal, “Buyer’s Medicinal Chemistry and Drug Discovery –Principles and practice” M.E Wolff, John Wiley & Sons Inc., New York, 1995
4. L.M. Artherden, “Text book of pharmaceutical chemistry”, Oxford University press, London, 1985

## **10CH311 INDUSTRIAL ELECTROCHEMISTRY**

**Credits 4:0:0**

**Course objective:**

- To know about metal finishing and synthesis of electrochemical inorganic / organic materials
- To learn about electrochemical powder sources and solar cells

**Outcome:**

- Students will get exposed to underlying electrochemical principles of metal finishing, electrochemical materials, electrochemical power sources and solar cells

**Unit I. Metal Finishing**

Electrodeposition potential, E.m.f series, Electroplating process, Faraday's laws, Anodes for plating, Effects of plating variables, Throwing power of the bath, General principles of surface preparation - Electroplating of copper, chromium, zinc and gold -Electroplating for electronic industry- Electroless plating of nickel- Anodizing – Electroforming.

**Unit II. Conducting Polymers and Electrochemicals**

Electropolymerisation- anodic and cathodic polymerization- effects of reaction parameters on the course of the reaction- Electrochemical preparation of conducting polymers- Electrolytic production of perchlorates and manganese dioxide - Electro-organic synthesis of adiponitrile and hydroquinone.

**Unit III. Batteries and Power Sources – I**

Principles of energy conservation- electrochemical energy conservation- thermodynamic reversibility, Gibb's equation, classification of batteries, types of electrolytes, battery characteristics, battery specifications, battery components, evaluation of battery performance.

**Unit IV. Batteries and Power Sources – II**

Construction and characteristics of primary batteries: Dry Leclanche cells, alkaline primary batteries and family of lithium batteries. Secondary batteries: Lead acid – car, traction, stationary, standby and sealed batteries. Nickel cadmium – pocket plates and sintered plates – vented and sealed maintenance free designs. Fuel cells- Introduction, types of fuel cells, advantages.

**Unit V. Solar cells: Material Science approach**

Principles and characteristics of Solar cells, Materials approach: fabrication of pure, polycrystalline, amorphous Si cells and thin film solar cells - CdS/Cu<sub>2</sub>S cells. Photo electrochemical cells (PEC) for conversion of light energy into electrical energy - PEC cells based on GaAs.

**Text books:**

1. D. Pletcher and F. C. Walsh, "Industrial electrochemistry", Chapman and Hall, London, 1990.
2. A. T. Khun, "Industrial Electrochemistry", Elsevier Publishers, 1972.
3. R. J. Wattman and J. Bargon, Can. J. Chem.64, 76 (1986)

**Reference books:**

1. N. V. Parthasarathy, "Practical Electroplating Handbook", Prentice-Hall, Inc. New Jersey, 1989.
2. M. M. Baizer, "Organic electrochemistry", Dekker Inc. New York, 1983.
3. M. R. Rifi and Frank. H. Covitz, "Introduction to Organic Chemistry", Dekkar Inc. New York, 1974.
4. M. Barak, "Electrochemical power sources", IEEE series, Peter Peregrinius Ltd, Steverage, U.K. 1980, reprinted during 1997.
6. G. S. Sodhi. "Environmental Chemistry", Narosa Publishing House Ltd, New Delhi, 2009.
7. David Linden, "Handbook of Batteries". Second edition. McGraw-Hill Inc, New York.
8. Venkatasubbiah, "Batteries", Efy Enterprises, Ltd, 1987.
9. K.L. Chopra and S. R. Das, "Thin film and solar cells", Plenum Press, New York, 1983.
10. Janne Halme, "Dye-Sensitised Nanostructured and Organic Photovoltaic cells", Master's Thesis.
11. H. P. Garag and J. Prakash, "Solar Energy: Fundamentals and Applications", Tata McGraw-Hill Publishing Company Ltd., New Delhi.
12. J. D. Coyle, R. R. Hill and D. R. Roberts (Eds) "A Source book in Photochemistry", Open University Press, U. K. 1982.
13. Bruno Scrosatti, "Applications of Electroactive polymers", Chapman & Hall, London, 1993.

**CHEMISTRY**

## ADDITIONAL SUBJECT

| Code    | Subject Name               | Credits |
|---------|----------------------------|---------|
| 10CH220 | Chemistry in Everyday Life | 4:0:0   |

### 10CH220 - CHEMISTRY IN EVERYDAY LIFE

**Credits: 4:0:0**

**Course Objective:** To understand the role of chemistry in everyday life

**Course Outcome:** The candidates will be familiar with the drugs and diseases, perfumes, explosives and dyes, chemicals in everyday products, chemical basis for everyday phenomena and knowing chemistry for better life.

#### **Unit – I: Drugs and diseases**

Clinical chemistry – antibiotics, antiseptics, antipyretics – definitions, examples (common drugs available in the market) – incurable diseases – causes for polio, diabetes, AIDS, cancer – signs and symptoms – vaccination – protein misfolding and disease – common drugs banned in India – effects of using banned drugs – effects of steroidal injections

#### **Unit – II: Perfumes, explosives and dyes**

Perfumes: historical significance – the olfactory system – categories – chemistry of ice cream making – chemistry of paint – chemistry of explosives – TNT, RDX, nitrocellulose, nitroglycerine (structure and properties only) – natural dyes and synthetic dyes – types, advantages, applications – hair dye – petrochemicals

#### **Unit – III: Chemicals in everyday products**

Advantages and disadvantages of the following: monosodium glutamate (aginomotto) – lycopene (in tomato) – umami, the fifth taste and glutamate – caffeine and theobromine (in chocolates) – polyphenols (in tea) – docosahexanoic acid (in fish) – thiols (in onion) – polycyclic aromatic hydrocarbons (formed during cooking meat) – constituents of talcum powder and pulmonary fibrosis – ingredients of tooth paste – melatonin (in anti-ageing product) – microban (in toys) – alpha tocopherol (in body lotions) – aluminum chloride (in antiperspirants) – aspartame (in artificial sweetener) – chloral hydrate (in sedatives) – citric acid (in citrus fruits)

#### **Unit – IV: Chemical basis of everyday phenomena**

Chemical basis of everyday phenomena – reasoning: kitchen gas burner burns yellow when a pot of boiling water overflows – cosmetic creams feel cool when applied to skin – seashells vary in color – old paintings discolor over time – hair color products remove gray on hair – disappearing inks disappear – water does not relieve the burning sensation of chilly – sniffing dogs detect explosives and bombs – flesh of fish smells different from other meat – puff pastries expand when prepared – some fabrics are water-repellent – cotton is highly water absorbent but dries slowly

### **Unit - V: Knowing chemistry for better life**

Food adulteration – consumption of alcohol and its ill effects – PAH from oil – balanced diet – iodized salt – fluoride tooth paste – saturated and unsaturated fat - cholesterol (LDL and HDL) – ill health and fast food – organic food – crackers – ill effects of crackers – molecules of emotion (Adrenaline , Acetylcholine , Dopamine, Epinephrine, Norepinephrine , Serotonin, Melatonin , Oxytocin)

#### **References:**

1. [www.listverse.com/2007/10/04/top-10-incurable-diseases/](http://www.listverse.com/2007/10/04/top-10-incurable-diseases/)
2. [www.bama.ua.edu/](http://www.bama.ua.edu/)
3. [www.foodproductdesign.com](http://www.foodproductdesign.com)
4. [www.angelfire.com/linux/chemistryofpaint/](http://www.angelfire.com/linux/chemistryofpaint/)
5. [www.srsi.org/sr1/weapon.explode.htm](http://www.srsi.org/sr1/weapon.explode.htm)
6. K.K. Karukstis and G.R.V. Hecke, Chemistry connections: the chemical basis of everyday phenomena, Ed. 2, Elsevier Science and Technology books, 2003
7. Paul Engel, Pain-free biochemistry, Wiley – Blackwell publishers, 2009
8. Grace Ross Lewis, 1001 Chemicals in everyday products, Ed. 2, John Wiley and sons, 1999

**DEPARTMENT OF  
CHEMISTRY**

## ADDITIONAL SUBJECT

| Subject Code | Subject Name                             | Credit |
|--------------|--|--------|
| 10CH312      | Natural Products and Medicinal Chemistry | 4:0:0  |

### 10CH312 - NATURAL PRODUCTS AND MEDICINAL CHEMISTRY

**Credit: 4:0:0**

**Course Objective:** To study the basics and important applications of natural products and medicinal chemistry.

**Course Outcome:** The candidates will be familiar with the basics of medicinal chemistry and natural products, drug targets, pharmacokinetics and anthocyanidins and pigments.

#### **Unit I: Basics of medicinal chemistry**

Brief history of medicinal chemistry – classification of drugs – brief description of biological, chemical, computer revolutions in drug design – pro drugs and soft drugs – design of pro drug system – multiple pro drug formation – soft drug principle and applications

#### **Unit II: Drug targets and drug solubility**

Enzymes and enzyme inhibitors – competitive and non-competitive inhibitors – reversible and irreversible inhibitors – ligand-receptor theories – Clark's theory and Paton's rate theory – proteins, lipids, and nucleic acids as drug targets – effect of pH,  $pK_a$ , and polarity on drug solubility

#### **Unit III: Pharmacokinetics and drug metabolism**

Natural resources of lead compounds – absorption, distribution, metabolism, and elimination – oxidation and hydrolysis – testing drugs in vitro – high-throughput screening – testing drugs in vivo – therapeutic index and therapeutic ratio

#### **Unit IV: Basics of Natural products**

Classification of natural products – classification based on chemical structure, physiological activity, taxonomy and biogenesis - classifications of amino acids – general methods of synthesis of amino acids – general reactions of amino acids (amino group and carboxyl group) – structure of peptides – structure and functions of DNA and RNA

#### **Unit V: Anthocyanidins and Pigments**

Introduction – structure of anthocyanidins – general methods of synthesizing anthocyanidins – Flavones: general methods of structure determination – synthesis of flavones and isoflavones – structure and reactions of flavonol and quercetin – biosynthesis of flavones – Tannins.

**References:**

1. Francis A. Carey, "Organic Chemistry", 5<sup>th</sup> edition, Tata McGraw Hill, New Delhi, 2003
2. Graham Solomons T.W, "Organic Chemistry", Vol. I & II, 5th Edn, John Wiley & Sons, New York, 1992
3. Bentley and Drivers, "Pharmaceutical Chemistry", Oxford University Press, London, 1985
4. Ashutosh Kar, "Medicinal Chemistry", Wiley Easter Ltd., Chennai, 1992
5. I.L. Finar, "Stereo chemistry and Chemistry of natural products", Volume 2, 5<sup>th</sup> edition, Longman company Ltd., London, 1991
6. D.J. Abraham, Burger's Medicinal Chemistry, 6<sup>th</sup> ed., Vol. 1-6; Ed. (RS403 .B8 2003 - vol.1-6)
7. Daniel Lednicer and Lester A. Mitscher, Organic Chemistry of Drug Synthesis, Vol. I-6, (RS 403.L38-vol. 1-6)
8. Joel G. Hardman, Lee L. Limbird and Alfred Gilman, Goodman & Gilman's the Pharmacological Basis of Therapeutics, 10<sup>th</sup> ed., (RM300 .G644), 2001

**ADDITIONAL SUBJECTS**

| Sub. Code | Name of the Subject          | Credits |
|-----------|------------------------------|---------|
| 11CH101   | APPLIED CHEMISTRY            | 3:0:0   |
| 11CH301   | INORGANIC CHEMISTRY – I      | 4:0:0   |
| 11CH302   | INORGANIC CHEMISTRY – II     | 4:0:0   |
| 11CH303   | INORGANIC CHEMISTRY – III    | 4:0:0   |
| 11CH304   | INORGANIC CHEMISTRY LAB      | 0:0:4   |
| 11CH305   | ORGANIC CHEMISTRY LABORATORY | 0:0:4   |
| 11CH306   | PHYSICAL CHEMISTRY LAB       | 0:0:4   |

**11CH101 APPLIED CHEMISTRY****Credits: 3:0:0****Course Objectives:**

- to understand the mechanism, properties and application of industrially important polymeric resin.
- to know the boiler problems associated with hardwater
- to understand the working principle of batteries and fuel cell
- to understand the working principle of smart materials and synthesis of nanomaterials.

**Course Outcome:** The students will come out with thorough knowledge of chemical principles involved in polymer, water technology, electrochemistry and in corrosion control. They will also know the various applications of variety of materials.

**Unit I: High Polymers**

Classification-functionality of polymer-mechanism (free radical, ionic and Zeigler-Natta)- Polymerisation-Plastics-thermoplastics and thermosetting plastics-compounding and fabrication of plastics-important thermoplastic resins-polyethylene(PE)-polyvinyl chloride (PVC)-important thermosetting plastic resins-phenolic resin and silicone resin- industrial polymers-nylons-epoxy resin-polyester resin-application of polymers-conducting polymers-semiconducting polymers.

**Unit II: Water Technology**

Sources of water-hardness of water-units of hardness-estimation of hardness-EDTA method and alkalinity method-softening of hard water-Lime Soda process-Zeolite process-demineralization or ion-exchange process-scale and sludge formation in boilers-internal conditioning-boiler corrosion-caustic embrittlement-desalination-water for drinking purpose.

**Unit III: Fuels and Combustion**

Fuels and classification-Gross and Net Calorific values-Proximate analysis and Ultimate analysis of coal- significances- characteristics of metallurgical coke-manufacture of coke by Otto-Hoffman method-synthetic petrol-Bergius process- Fischer-Tropsch process-Knocking-octane number-cetane number-improvement of anti-knocking characteristics, gaseous fuels-an elementary treatment of water gas, producer gas and CNG (definition only)- an introduction to non-conventional sources of energy-bio fuels (biodiesel and bioethanol)-theoretical calculation of calorific values (Dulong's formula)-simple problems-calculation of minimum air requirements-simple problems-Flue gas analysis-Orsat's apparatus.

**Unit IV: Electrochemistry**

Electrode potential-measurement of electrode potential-Nernst equation for electrode potential-electrochemical series-electrochemical cell or Voltaic cell-Concentration cell-Primary cell-Leclanche cell-Secondary batteries- alkaline batteries-lead acid and Lithium batteries – An introduction to fuel cell, H<sub>2</sub>-O<sub>2</sub> Fuel cell- Applications - Types of corrosion - Wet or electrochemical corrosion- Types – Factors influencing corrosion-Corrosion control methods.

**Unit V: Materials and Nanomaterials**

Introduction to ceramic materials, biomaterials and smart materials- preparation, properties and applications: Alumina (Al<sub>2</sub>O<sub>3</sub>), Silica (SiO<sub>2</sub>), Hydrogel, Calcium hydroxyl apatite, Barium Titanate, Lead zirconate titanate, Nitinol and Cu-Al-Be alloy.

Introduction to nanomaterials-classification: bottom up and Top down approaches: sol-gel method, self assembled monolayer method and ball milling method.

**Text books**

1. A text book of engineering chemistry by P.C.Jain and Monica Jain, Dhanapat Rai publications, New Delhi, 12<sup>th</sup> ed., 2006.
2. Engineering Chemistry by Dr.B.S.Chauhan, Laxmi publication, 3<sup>rd</sup> ed, 2009.

**Reference books**

1. Nano: The essentials: Understanding Nanoscience and Nanotechnology, T.Pradeep, McGraw-Hill Professional publishing, 2008.
2. Smart materials by Tawee Tunkasiri, Trans Tech Pubn, 2008.
3. Ceramic Materials: Process. Properties and application by Philippe Boch and Jean claude, Herms science publication, 2001.
4. Biomaterial Science by Buddy D.Ratner, Allan S.Hoffman, Fraderick T.Schoen and Jack E.Lemons, Academic Press, 1996.

**11CH301 INORGANIC CHEMISTRY – I**

**Credits: 4:0:0**

**Course Objectives:**

- The various bonding theories in inorganic chemistry will be discussed
- Background on inorganic chemistry as applied to solid state chemistry will be discussed.
- The student will study the detailed account of nuclear chemistry and their application in various fields
- The student will understand the principles of metallurgy and will study the importance of lanthanides and actinides in detail

**Course Outcome:**

- The student will get the thorough knowledge of various bond theories, solid state chemistry, Nuclear chemistry, metal extraction techniques and the various properties of lanthanides and actinides

**Unit I : Structure and Bonding**

**Ionic bond** – Formation – Characteristics of ionic compounds: melting point, boiling point, hardness, electrical conductivity and solubility – Structure of crystal lattices – Lattice energy: Born-Lande equation and Born Heber Cycle – Polarisation of ions: Fajan's rule – Calculation of some limiting ratio values – **Covalent bond** – Rules for covalent bond formation – Valence bond theory – Resonance and hybridization – Molecular orbital theory and its application in diatomic molecules – Comparison of VB and MO theories – Bond properties – Bond energy – Bond length – Bond polarity – Electron pair repulsion theory and its applications – **Hydrogen bond** – Types – Effect on molecular properties – Detection of hydrogen bonding.

**Unit II : Solids**

Bond theory of solids – Electrical properties – Insulators – Semiconductors – Superconductors – Dislocation in solids – Schottky and Frenkel defects – Structure of some compounds of AX, AX<sub>2</sub> and AmX<sub>2</sub> types – Perovskite, Ilmenite and Spinel structures

**Unit III : Nuclear Chemistry**

Modes of radioactive decay and rate of radioactivity decay – Radioactive detectors – Types of nuclear reactions – Artificial radioactivity – Nuclear stability – Packing fraction – Mass defects and binding energy – Nuclear fission of uranium - Liquid drop model – Nuclear fusion – Essential features of water cooled thermal reactors and fast breeders – Neutron activation analysis – Carbon and rock dating – Applications of tracers in chemical analysis, reaction mechanisms, medicine and industry

**Unit IV: Metallurgy**

Isolation, purification, properties and uses of Beryllium, Germanium, Titanium, Zirconium, Thorium, Vanadium, Uranium and Platinum. – Preparation and uses of the following compounds: Basic Beryllium acetate, BeCl<sub>2</sub>, TiCl<sub>4</sub>, TiO<sub>2</sub>, Titanium isopropoxide, ZrCl<sub>4</sub>, Zirconia, V<sub>2</sub>O<sub>5</sub>, VCl<sub>4</sub>, UF<sub>4</sub>, Uranyl nitrate, ThO<sub>2</sub>, Th(NO<sub>3</sub>)<sub>2</sub>, PtCl<sub>4</sub>, H<sub>2</sub>PtCl<sub>6</sub>

**Unit V: Chemistry of Lanthanides and Actinides**

Lanthanides – Position in the periodic table – General properties of lanthanides and actinides – Electronic configuration, oxidation state and oxidation potential, atomic and ionic radii – Cause and consequences of lanthanide and actinide contractions – Comparison of spectral and magnetic properties of lanthanide and actinide complexes – Chemistry of their important compounds: Oxides, nitrates and sulphates

**Text Books:**

- F. A. Cotton and G. Wilkinson, “Advanced Inorganic Chemistry”, 6th edition, Wiley India (P.) Ltd, New Delhi, India, First Reprint 2007
- J. D. Lee, “Concise Inorganic Chemistry”, 5th edition, Wiley India (P.) Ltd, New Delhi, India, Reprint:2009

**Reference Books:**

- Shriver and Atkins, “ Inorganic Chemistry”, 4<sup>th</sup> edition, Oxford University Press, New Delhi, India, 2009
- N. N. Greenwood and A. Earnshaw, “Chemistry of the Elements”, 2<sup>nd</sup> edition, Reed Elsevier India Private Ltd, Gurgaon, India, Reprinted 2010
- R. West, “Solid State Chemistry and its Applications”, Wiley India Pvt. Ltd, New Delhi, India, 2007
- H. J. Arnikar, “Essentials of Nuclear Chemistry”, 4th edition, New Age International Publishers Ltd., New Delhi, India, 2007

**11CH302 INORGANIC CHEMISTRY – II**

**Credits: 4:0:0**

**Course Objectives:**

- Coordination Chemistry is the backbone of inorganic chemistry and the structure and reaction mechanisms of coordination complexes will be discussed
- The various reaction mechanisms including substitution, electro-transfer and photochemical reactions will be discussed

- The importance of main group chemistry will be discussed

**Course Outcome:**

- The student will get the thorough knowledge about the coordination chemistry. He will understand the various bonding theories in inorganic complexes and the types of mechanisms involved in coordination chemistry. He will also know the importance of main group chemistry.

**Unit I: Coordination Chemistry – Structure and Bonding**

Introduction - Formation of complexes - Bonding theories for coordination complexes – **Werner's theory** – Stability constant: Experimental determination of stability constant – Factors influencing – Stabilization of unusual oxidation states by complex formation – **Crystal field theory** – concept, influence of ligand on CF splitting and limitation – Term symbols – Orgel diagram– Tanabe Sugano diagrams ( $d^1$  and  $d^2$ ) - Ligand field theory – Jahn – Teller effect – Electronic spectra and magnetic moments - types of magnetic interactions -Recent techniques of magnetic susceptibility measurements - Low-spin – high-spin transitions - **Molecular orbital theory** of a complex and its limitation – Ligand Design – Chelate and macrocyclic Effect - Isomerism in Metal Complexes – Optical isomerism - Stereochemical nonrigidity

**Unit II : Inorganic Reaction Mechanisms – Substitution Reactions**

Reactions of square – planar complexes – Mechanism of ligand displacement reaction – Substitution in the square planar complexes - Mechanism, entering group effect, cis effect and trans effect - Thermodynamic and kinetic stability -Substitution in octahedral complexes – Dissociative and associative mechanisms – Base hydrolysis - Isomerisation reactions – Substitution without breaking the metal –ligand bond

**Unit III : Inorganic Reaction Mechanisms – Electron Transfer Reactions**

Electron transfer reactions – Outer sphere and inner sphere mechanisms and rate laws - Various types of electron transfer reactions - Marcus-Husch theory Correlation between thermal and optical electron transfer reactions - Identification of intervalence transfer bands in solution

**Unit IV: Inorganic Photochemistry**

Excited states of Coordination complexes - Properties of excited states - Photochemical pathways - Energy transfer, Charge transfer photochemistry, Photoredox reactions, Photosubstitution reactions - Ruthenium polypyridines - Ligand photoreactions - Photochemical conversion and storage of solar energy – Introduction to inorganic photochemistry at semiconductor electrodes

**Unit V : Main Group Chemistry**

Preparation, structure and bonding of boron hydrides, carboranes and heteroboranes - Polymorphism of carbon, phosphorous and sulphur – Synthesis, structures and properties of silicates and carbides - Oxyacids of selenium and tellurium - Chalcogenide clusters - Homocyclic inorganic systems

**Text Books:**

- J. E. Huheey, E. A. Keiter and R. L. Keiter, “Inorganic Chemistry – Principles of structure and reactivity” 4th edn., Dorling Kindersley (India) Pvt. Ltd, New Delhi, India, 2009
- W. W. Porterfield, “Inorganic Chemistry A Unified Approach” 2<sup>nd</sup> Edition, Reed Elsevier India Private Ltd, Gurgaon, India, Reprinted 2009

**Reference Books:**

- F.A. Cotton and G. Wilkinson, "Advanced Inorganic Chemistry", 6th edition, Wiley India (P.) Ltd, New Delhi, India, First Reprint 2007
- G. L. Miessler and D. A. Tarr, "Inorganic Chemistry", 3rd Edition., Dorling Kindersley (India) Pvt. Ltd, New Delhi, India, 2009
- B. E. Douglas, D. H. McDaniel and J. J. Alexander, "Concepts and Models of Inorganic Chemistry", 3<sup>rd</sup> edition, Wiley India (P.) Ltd, New Delhi, India, Reprint 2007
- B. N. Figgis and M. A. Hitchman, "Ligand Field Theory and Its Applications", Wiley-VCH Verlag GmbH & Co, Weinheim, Germany, 2000
- R. B. Jordan, "Reaction Mechanisms of Inorganic and Organometallic Systems", 3<sup>rd</sup> Edition, Oxford University Press, New York, USA, 2007
- M. Driess, H. Nöth, "Molecular Clusters of the Main Group Elements", Wiley-VCH Verlag GmbH & Co, Weinheim, Germany, 2004

### 11CH303 INORGANIC CHEMISTRY – III

**Credits: 4:0:0**

#### **Course Objectives:**

- The frontier areas in inorganic chemistry will be discussed
- The application of organometallic complexes in various fields and the role of metals in biology will be discussed
- The student will study the detailed account of inorganic polymers.
- The role of metals in nanotechnology and the importance of various nanoparticles and their application will be discussed.

#### **Course Outcome:**

- The student will get the thorough knowledge about the nonaqueous solvents, the synthesis and application of organometallic complexes and the importance of bioinorganic chemistry, the use of inorganic polymers and the importance of inorganic chemistry in nanotechnology.

#### **Unit I: Nonaqueous Solvents**

General properties and classification of solvents – Self-ionization and leveling effect – Reactions in nonaqueous solvents – Solute-solvent interaction - Reactions in liquid NH<sub>3</sub> – Solutions of metals in liquid ammonia – Reactions in acetic acid, anhydrous sulphuric acid, liquid SO<sub>2</sub>, liquid HF, interhalogens and liquid dinitrogen tetroxide – Titrations in nonaqueous solvents – Acid-base titrations.

#### **Unit II : Organometallics**

Definition – Types of bonds – Metal carbonyls – Metal Nitrosyls - Complexes of olefin, acetylene, cyclopentadiene and benzene derivatives – Metallocenes – Fluxional molecules – Reactions – Coordinative unsaturation - Substitution, Oxidative addition, Reductive elimination, Insertion - Reactions of coordinated ligand – Catalysis: Hydrogenation, Carbonylation, Hydroformylation, Wacker Process and Ziegler-Natta Catalysis

#### **Unit III : Bio-inorganic Chemistry**

Essential and trace metals in biological systems – Metalloporphyrins – Chlorophyll, hemoglobin, myoglobin and vitamin B<sub>12</sub> – Iron sulphur proteins – Hydrogenase - Nitrogen cycle, nitrogen fixation and dinitrogen complexes – Metal centered enzymes – structure and function – Role of metal complexes in medicine: anticancer drugs (Pt complexes and their mechanism of action).

#### **Unit IV: Inorganic Polymers**

Classification, Types of Inorganic Polymerization - Comparison with organic polymers – Structure, properties and uses of inorganic polymers - Boron-oxygen and boron-nitrogen polymers –

**Unit V: Nanomaterials**

General introduction - Synthesis of nanoparticles of gold and silver - Synthesis of nanoparticle semiconductors ( $\text{TiO}_2$  and  $\text{Fe}_2\text{O}_3$ ) - Nanowires and nanorods - Self-assembled nanostructures: Self-assembly and bottom-up fabrication – Graphenes, fullerenes and nanotubes - Applications of nanoparticles.

**Text books:**

- F.A. Cotton and G. Wilkinson, “Advanced Inorganic Chemistry”, 6th edition, Wiley India (P.) Ltd, New Delhi, India, First Reprint 2007
- B. R. Puri, L. R. Sharma and K. C. Kalia, “Principles of Inorganic Chemistry”, 31<sup>st</sup> Edition, Milestone Publishers and Distributors, New Delhi, India, 2008

**Reference books:**

- J. E. Huheey, E. A. Keiter and R. L. Keiter, “Inorganic Chemistry – Principles of structure and reactivity” 4th edn., Dorling Kindersley (India) Pvt. Ltd, New Delhi, India, 2009
- Shriver and Atkins: “Inorganic Chemistry”, 4<sup>th</sup> edition, Oxford University Press, New Delhi, India, 2009
- B. D. Gupta and A .J. Elias, “Basic Organometallic Chemistry”, CRC Press, New Delhi, India, 2010
- I. Bertini, H. B. Gray, S. J. Lippard, J. S. Valentine, “Bioinorganic Chemistry”, Viva Books Private Ltd, New Delhi, India, 2007
- R. D. Archer, “Inorganic and Organometallic Polymers”, John Wiley and Sons, New York, USA, 2001
- G.Zhong Cao. “Nanostructures and Nanomaterials: Synthesis, Properties and Applications”, Imperial College Press, London, United Kingdom, 2004

**11CH304 INORGANIC CHEMISTRY LAB****Credits: 0:0:4****Course Objectives:**

- To provide the students an appreciation for the synthesis of Inorganic Complexes
- To provide the students a competence in the laboratory skills required for accurate and precise chemical analysis
- The students will know the theoretical basis of qualitative inorganic analysis containing common and less common ions

**Course Outcome:**

- The student will gain the laboratory skills to synthesize the inorganic complexes, to estimate the amount of metals quantitatively by complexometric and redox titrations and will be confident in analyzing the mixtures containing common and less common ions using semimicro analysis

Totally 20 experiments will be done

|   |         |
|---|---------|
| (Inorganic complex preparations                                   | = 6,    |
| Complexometric, redox titrations                                  | = 6 and |
| Inorganic analysis containing two common and two less common ions | = 8)    |

**Inorganic complex Preparations (Any six)**

- Hexathiourea Lead (II) nitrate
- Trithiourea Copper(II) chloride dehydrate
- Pentakis(thiourea) dicopper(I) nitrate dehydrate
- Potassiumtrioxalato ferrate (III)
- Bisglycinatecopper(II) monohydrate
- Hexamminecobalt(III) chloride
- Chloropentaamminecobalt (III) chloride
- Nitritopentamminecobalt (III) chloride
- Nitropentamminecobalt (III) chloride

**Titration (Any six)**

- Estimation of Zinc by EDTA titrations
- Estimation of Calcium by EDTA titrations
- Estimation of Nickel by EDTA titrations
- Estimation of  $\text{Fe}^{2+}$  using redox titrations
- Estimation of Aluminium by EDTA titration (Back titration)
- Estimation of Nickel by EDTA titration (Back titration)
- Estimation of Lead by EDTA titration
- Estimation of Chromium by redox titrations

**Inorganic Qualitative Analysis**

There will be 8 inorganic qualitative analysis experiments containing two common and two less common ions.

**Text Books**

- J. Mendham, R. C. Denny, J. D. Barnes and M. J. K. Thomas, "Vogel's textbook of quantitative chemical analysis", 6<sup>th</sup> edition, Dorling Kindersley (India) Pvt. Ltd, New Delhi, India, Seventh impression 2008
- V. V. Ramanujam, "Inorganic semimicro qualitative analysis", 3<sup>rd</sup> edition, The national publishing company, Chennai, India, reprinted 2008

**Reference Book**

- G. Svehla, "Vogel's textbook of qualitative chemical analysis", 6<sup>th</sup> edition, Dorling Kindersley (India) Pvt. Ltd, New Delhi, India, fifth impression 2008

**11CH305 ORGANIC CHEMISTRY LABORATORY EXPERIMENTS**

**Credits: 0:0:4**

**Course Objective:** To enrich the knowledge of Organic Laboratory skills for single step preparation, estimation and analysis of Organic mixture.

**Course Outcome:** Students acquire the knowledge of synthesis, estimation and analysis of Organic Compounds.

**Experiment A: Single Step Preparation**

1. Preparation of Acetanilide From aniline (Acetylation)
2. Preparation of sSalicylic acid from Methyl-salicylate (Hydrolysis)
3. Preparation of bromoacetanilide from acetanilide (Bromination)
4. Preparation of p-nitroacetanilide from acetanilide (Nitration)

5. Preparation of Picric acid from Phenol (Nitration)
6. Preparation of benzanilide from aniline (Benzoylation)

**Experiment B: Estimation**

1. Estimation of aniline
2. Estimation of Phenol
3. Estimation of Dimethylketone
4. Estimation of Ascorbic acid
5. Estimation of Glucose (Bertrand's method)
6. Estimation of Saponification value of oil

**Experiment C: Separation of Binary mixture and Analysis**

Six experiments will be conducted with six different binary mixtures

**11CH306 - PHYSICAL CHEMISTRY LAB**

**Credits: 0:0:4**

**Course Objective**

To carryout simple chemical reaction which would be monitored by Electrical and Non-Electrical experimental studies.

**Course Outcome**

The analytical skill will be improved by pursuing electrical experiments like Conductometry, Spectrophotometry, Potentiometry.

The basic knowledge could be understood thoroughly regarding the velocity of the reaction, distribution properties and adsorption studies.

**ELECTRICAL EXPERIMENTS**

1. Determination of Standard Electrode Potential.
2. Determination of solubility and solubility product of sparingly soluble salt.

**ACID-BASE TITRATION – CONDUCTOMETRY**

3. Strong base Vs Strong acid
4. Strong base Vs mixture of Strong and Weak acids

**REDOX TITRATIONS -- POTENTIOMETRY**

5. Potassium Dichromate Vs Ferrous Ammonium Sulphate
6. Potassium Permanganate Vs Ferrous Ammonium Sulphate

**PRECIPITATION TITRATION -- POTENTIOMETRY**

7. Silver Nitrate Vs Potassium Chloride
8. Silver Nitrate Vs mixture of Halides

**NON-ELECTRICAL EXPERIMENTS**

9. Determination of distribution coefficient and equilibrium constant of  
 $KI + I_2 \rightleftharpoons KI_3$
10. Phase diagram – Simple Eutectic System.

11. Phase diagram – Compound formation.

**KINETICS EXPERIMENTS**

12. Ester Hydrolysis – Comparison of acid strength
13. Ester Hydrolysis – Verification of Arrhenius equation

**ADSORPTION ISOTHERM**

14. Freundlich Adsorption Isotherm – Verification

**SPECTROPHOTOMETRY**

15. Estimation of Chromium – Verification of Beer's Law

## LIST OF SUBJECTS

| Sub. Code | Name of the Subject                                   | Credits |
|-----------|---|---------|
| 11CH201   | Chemistry in Everyday Life                            | 3:0:0   |
| 12CH201   | Applied Chemistry                                     | 3:0:0   |
| 12CH202   | Applied Chemistry Lab                                 | 0:0:2   |
| 12CH203   | Environmental Studies                                 | 3:0:0   |
| 12CH204   | Physical Chemistry                                    | 4:0:0   |
| 12CH205   | Principles of Organic Chemistry                       | 3:0:0   |
| 12CH206   | Inorganic and Co-ordination chemistry                 | 4:0:0   |
| 12CH207   | Organic reactions and mechanisms                      | 4:0:0   |
| 12CH208   | Materials Chemistry                                   | 4:0:0   |
| 12CH209   | Biochemistry  | 3:0:0   |
| 12CH210   | Characterization and instrumental techniques          | 4:0:0   |
| 12CH211   | Medicinal Chemistry                                   | 4:0:0   |
| 12CH212   | Analytical Chemistry and Spectroscopy                 | 4:0:0   |
| 12CH213   | Supramolecular Chemistry                              | 4:0:0   |
| 12CH214   | Cheminformatics                                       | 4:0:0   |
| 12CH215   | Qualitative analysis and inorganic preparations Lab   | 0:0:2   |
| 12CH216   | Organic qualitative analysis Lab                      | 0:0:2   |
| 12CH217   | Titrimetric analysis and gravimetric analysis Lab     | 0:0:2   |
| 12CH218   | Physical chemistry Lab                                | 0:0:2   |
| 12CH219   | Synthesis of organic compounds and chromatography Lab | 0:0:2   |
| 12CH220   | Chemistry in Everyday Life                            | 3:0:0   |
| 12CH301   | Organic Chemistry – I                                 | 4:0:0   |
| 12CH302   | Physical Chemistry – I                                | 4:0:0   |
| 12CH303   | Inorganic Chemistry – I                               | 4:0:0   |
| 12CH304   | Organic Chemistry – II                                | 4:0:0   |
| 12CH305   | Physical Chemistry – II                               | 4:0:0   |
| 12CH306   | Inorganic Chemistry – II                              | 4:0:0   |
| 12CH307   | Organic Chemistry – III                               | 4:0:0   |
| 12CH308   | Physical Chemistry – III                              | 4:0:0   |
| 12CH309   | Inorganic Chemistry – III                             | 4:0:0   |
| 12CH310   | Inorganic Chemistry Lab                               | 0:0:4   |
| 12CH311   | Organic Chemistry Lab                                 | 0:0:4   |
| 12CH312   | Physical Chemistry Lab                                | 0:0:4   |
| 12CH313   | Analytical Chemistry – I                              | 4:0:0   |
| 12CH314   | Analytical Chemistry – II                             | 4:0:0   |
| 12CH315   | Polymer Chemistry                                     | 4:0:0   |
| 12CH316   | Advanced Pharmaceutical Chemistry                     | 4:0:0   |
| 12CH317   | Industrial Electrochemistry                           | 4:0:0   |
| 12CH318   | Environmental Electrochemistry                        | 4:0:0   |
| 12CH319   | Molecular and Materials Self-assembly                 | 4:0:0   |
| 12CH320   | Chemical Approach to Nanomaterials                    | 4:0:0   |
| 12CH321   | Molecular Machines and Materials                      | 4:0:0   |
| 12CH322   | Nanotechnology in Fuel Cells and Energy Storage       | 4:0:0   |
| 12CH323   | Literature Survey                                     | 0:0:2   |

## 11CH201 CHEMISTRY IN EVERYDAY LIFE

Credits 3:0:0

### Course Objective:

- To introduce to the students about the chemistry connections of everyday life.
- To relate what the student studies in the subjects to practical life.

### Course Outcome:

- The students will know the practical aspects of chemistry in day-to-day life.
- The students will think innovative and develop application oriented products.

### Unit 1

**DRUGS AND DISEASES:** Clinical chemistry – antibiotics, antiseptics, antipyretics – definitions, examples (common drugs available in the market) – incurable diseases – causes for polio, diabetes, AIDS, cancer – signs and symptoms – vaccination – protein misfolding and disease – common drugs banned in India – effects of using banned drugs – effects of steroidal injections.

### Unit 2

**PERFUMES, EXPLOSIVES, AND DYES:** Perfumes: historical significance – the olfactory system – categories – chemistry of ice cream making – chemistry of paint – chemistry of explosives – TNT, RDX, nitrocellulose, nitroglycerine (structure and properties only) – natural dyes and synthetic dyes – types, advantages, applications – hair dye – petrochemicals.

### Unit 3

**CHEMICALS IN EVERYDAY PRODUCTS:** Advantages and disadvantages of the following: monosodium glutamate (aginomotto) – lycopene (in tomato) – umami, the fifth taste and glutamate – caffeine and theobromine (in chocolates) – polyphenols (in tea) – docosahexanoic acid (in fish) – thiols (in onion) – polycyclic aromatic hydrocarbons (formed during cooking meat) – constituents of talcum powder and pulmonary fibrosis – ingredients of tooth paste – melatonin (in anti-ageing product) – microban (in toys) – alpha tocopherol (in body lotions) – aluminum chloride (in antiperspirants) – aspartame (in artificial sweetener) – chloral hydrate (in sedatives) – citric acid (in citrus fruits).

### Unit 4

**CHEMICAL BASIS OF EVERYDAY PHENOMENA:** Chemical basis of everyday phenomena – reasoning: kitchen gas burner burns yellow when a pot of boiling water overflows – cosmetic creams feel cool when applied to skin – seashells vary in color – old paintings discolor over time – hair color products remove gray on hair – disappearing inks disappear – water does not relieve the burning sensation of chilly – sniffing dogs detect explosives and bombs – flesh of fish smells different from other meat – puff pastries expand when prepared – some fabrics are water-repellent – cotton is highly water absorbent but dries slowly.

### Unit 5

**KNOWING CHEMISTRY FOR BETTER LIFE:** Food adulteration – consumption of alcohol and its ill effects – PAH from oil – balanced diet – iodized salt – fluoride tooth paste – saturated and unsaturated fat - cholesterol (LDL and HDL) – ill health and fast food – organic food –

crackers – ill effects of crackers – molecules of emotion (Adrenaline, Acetylcholine, Dopamine, Epinephrine, Norepinephrine, Serotonin, Melatonin, Oxytocin).

### Text Books

1. Karukstis K.K., and Hecke G.R.V., “Chemistry connections: the chemical basis of everyday phenomena” Elsevier Science and Technology books, 2nd edition, 2003.
2. Grace Ross Lewis, “1001 Chemicals in everyday products”, John Wiley and sons, 3rd edition, 2001.

### References

1. [www.listverse.com/2007/10/04/top-10-incurable-diseases/](http://www.listverse.com/2007/10/04/top-10-incurable-diseases/)
2. [www.bama.ua.edu/](http://www.bama.ua.edu/)
3. [www.foodproductdesign.com](http://www.foodproductdesign.com)
4. [www.angelfire.com/linux/chemistryofpaint/](http://www.angelfire.com/linux/chemistryofpaint/)
5. [www.srsi.org/sr1/weapon.explode.htm](http://www.srsi.org/sr1/weapon.explode.htm)
6. Paul Engel, “Pain-free Biochemistry”, Wiley – Blackwell publishers, 2009.

## 12CH201 APPLIED CHEMISTRY

**Credits: 3:0:0**

### Course Objective:

- To understand problems associated with hard water and treatment methods.
- To learn about fabrication of polymers, industrially important polymers and their biodegradability.
- To know about calorific value of fuels, methods to improve anti-knocking characteristics, bio-fuels and flue gas analysis.
- To have understanding about construction and working of batteries, corrosion – types and control methods.
- To impart the basic aspects of inorganic engineering materials.

### Course outcome:

- To suggest methods to minimize problems related to hard water in industrial operations.
- To select and use eco-friendly fuels and biodegradable polymers for industrial and domestic purpose.
- To use appropriate methods to minimize corrosion of metals.

### Unit I

**WATER TECHNOLOGY:** Sources of water-hardness of water-units of hardness-estimation of hardness-EDTA method and alkalinity method-softening of hard water-Cold and Hot Lime Soda process-Zeolite process-demineralization or ion-exchange process-scale and sludge formation in boilers-internal conditioning-colloidal, phosphate, calgon, carbonate, complexometric conditioning, boiler corrosion-caustic embrittlement - desalination - Electro dialysis, reverse Osmosis-water for drinking purpose.

### Unit II

**HIGH POLYMERS:** Nomenclature-Functionality-Tacticity -Types of Polymerisation-addition, condensation, co-polymerisation, Plastics-thermoplastics and thermosetting plastics-

compounding – ingredients used in preparation of plastics, fabrication of plastics-compression, injection, extrusion, foaming, fibre-reinforced plastics, preparation, properties and uses of important thermoplastic resins-polyethylene(PE)-polyvinyl chloride (PVC)-important thermosetting plastic resins-phenolic resin and silicone resin- industrial polymers-nylons-epoxy resin-polyester resin- Rubber - vulcanization of rubber, Biodegradable polymers – definition and examples.

### **Unit III**

**FUELS AND COMBUSTION:** Fuels – classification, Combustion - Gross and Net Calorific values (Dulong’s formula) - calculation of air quantities - simple problems - Flue gas analysis-Orsat’s apparatus – Solid fuels – Coal-Proximate analysis and Ultimate analysis - significance-Metallurgical coke – carbonisation (definition) -characteristics of metallurgical coke-manufacture of coke by Otto-Hoffman method-Liquid fuels -synthetic petrol-cracking (definition)-Knocking-octane number -improvement of anti-knocking characteristics, cetane number, Gaseous fuels-Manufacture of water gas - CNG, LPG –definition, Biogas and biofuels, Rocket propellant – types.

### **Unit IV**

**ELECTROCHEMISTRY:** Electrode potential-measurement of electrode potential-Nernst equation for electrode potential-electrochemical series-electrochemical cell or Voltaic cell-Concentration cell-Primary cell-Leclanche cell-Secondary batteries- alkaline batteries-lead acid battery – Fuel cell –  $H_2-O_2$  Fuel cell – Corrosion -types – Chemical corrosion – oxidation corrosion, corrosion by other gases, liquid metal corrosion, electrochemical corrosion- types – galvanic corrosion, concentration cell corrosion, pitting corrosion, waterline corrosion - Factors influencing corrosion-Corrosion control methods.

### **Unit V**

**ENGINEERING MATERIALS:** Refractories – classification – requisite properties - Manufacturing steps- common refractories -silica bricks, dolomite bricks - Abrasives – properties- classification – synthetic abrasive – silicon carbide, boron carbide – preparation and uses – applications – Insulators – characteristics – electrical insulating materials – thermal insulators – classification - properties – Lubricants – Friction and wear, functions of lubricant – classification of lubricants – lubricating oils – semi solid lubricants – solid lubricants – selection of lubricants.

### **Text Books**

1. Jain P. C, Monica Jain, “A text book of engineering chemistry”, Dhanapat Rai publications, New Delhi, 12th edition, 2006.
2. Subha Ramesh, Vairam, Anandhan, “Engineering Chemistry”, Wiley India Pvt. Ltd., New Delhi, 2011.

### **Reference Books**

1. Gowrikar V. R, Viswanathan N. V, Jaydev Sreedhar, “Polymer Science”, New Age International Pvt. Ltd., New Delhi, 2000.
2. Agarwal C. V, “Chemistry of Engineering materials”, C.V. Tara Book Agency, 1982.
3. Shashi Chawla, “A text book of engineering chemistry”, Dhanapat Rai publications, New Delhi, 8th edition, 2008.
4. Palanna O. G, “Engineering Chemistry”, Tata McGraw Hill Education pvt., Ltd., New Delhi, 2009.

## 12CH202 APPLIED CHEMISTRY LAB

**Credits: 0:0:2**

### Course Objective:

- To train the students in gaining hands on experience to handle various applied chemistry laboratory techniques.

### Course Outcome:

- The students can apply their theoretical applied chemistry knowledge in practical applications.

### List of Experiments:

1. Estimation of sodium hydroxide.
2. Estimation of  $\text{Fe}^{2+}$  ions.
3. Estimation of Total, Permanent and Temporary hardness by EDTA method.
4. Estimation of Alkalinity in water sample.
5. Estimation of dissolved oxygen in water sample.
6. Estimation of Copper in Brass
7. pH Measurements for Acid/Alkali Titration.
8. Conductametric estimation of an acid.
9. Potentiometric estimation of  $\text{Fe}^{2+}$  ions.
10. Estimation of iron in water sample by spectro photometry.
11. Determination of Single Electrode Potential by Potentiometry.
12. Estimation of sodium / calcium / potassium metal ions present in water by flame photometer.

### Text Book

1. Mendhem J., Denny R. C., Barnes J. D., Thomas M. J. K., Vogel's Quantitative Chemical Analysis , Pearson Education limited, 6th Edition, 2000.

## 12CH203 ENVIRONMENTAL STUDIES

**Credits: 3:0:0**

### Course Objective:

- To acquire knowledge of elements of environment, it's need & importance.
- To know about pollution problems and green technology.
- To develop a sense of responsibility about the role of students in fostering the idea of learning to live in harmony with nature.
- To create an awareness about the major environmental issues for a sustainable development.

### Course Outcome:

- At the end of this course the students are expected to understand the importance of environment, the effect of technology on the environment and ecological balance and make them sensitive to the environment problems in every professional endeavor in which they participates.

## **Unit I**

**ENVIRONMENT AND NATURAL RESOURCES:** Environment - Definition, scope and importance, Renewable and Non-Renewable Resources – Natural resources and associated problems – Forest resources: Use and over-exploitation, deforestation, case studies. Timber extraction, mining, dams and their effects on forests and tribal people – Water resources: Use and over-utilization of surface and ground water, floods, drought, conflicts over water, dams-benefits and problems – Energy resources: Growing energy needs, renewable and non-renewable energy sources, and use of alternate energy sources. Case studies – Land resources: Land as a resource, land degradation, man induced landslides, soil erosion and desertification – Role of an individual in conservation of natural resources – Activity: Field study of local area to document environmental assets.

## **Unit II**

**ECOSYSTEMS AND BIODIVERSITY:** Concept of an ecosystem – Structure and function of an ecosystem – Producers, consumers and decomposers – Energy flow in the ecosystem – Ecological succession – Food chains, food webs -Introduction to Biodiversity – Definition: genetic, species and ecosystem diversity – Bio geographical classification of India – Value of biodiversity: consumptive use, productive use, social, ethical, aesthetic and option values – Biodiversity at global, National and local levels -Hot-spots of biodiversity – Threats to biodiversity: habitat loss, poaching of wildlife, man-wildlife conflicts – Endangered and endemic species of India – Conservation of biodiversity: In-situ and Ex-situ conservation of biodiversity – Activity: Model preparation for Ecosystems / Biodiversity - Documentation of available ecosystems – Biodiversity within Campus.

## **Unit III**

**ENVIRONMENTAL POLLUTION:** Definition, Causes, effects and control measures (two) – Air pollution (Cyclone separator, Electrostatic Separator) – Water pollution – Soil pollution – Noise pollution – Thermal pollution – Nuclear hazards – Solid waste management: Causes, effects and control measures of urban and industrial wastes – Role of an individual in prevention of pollution. Pollution case studies – Green chemistry– principles of sustainable and green chemistry Activity: Visit-nearby Sewage treatment Water Plant.

## **UNIT IV**

**SOCIAL ISSUES AND ENVIRONMENTAL LEGISLATION:** From Unsustainable to Sustainable development – Urban problems related to energy – Water conservation, rain water harvesting and watershed management –Environmental ethics: Issues and possible solutions – Climate change, global warming, acid rain, ozone layer depletion, case studies – Environment Production Act – Air (Prevention and Control of Pollution) Act – Water (Prevention and control of Pollution) Act – Wildlife Protection Act – Forest Conservation Act – Issues involved in enforcement of environmental legislation – Public awareness – Activity: Watching Documentary Movies & Video Clips related to environment problems – Social issues and control measures.

## **Unit V**

**HUMAN POPULATION AND THE ENVIRONMENT:** Population growth, Population explosion—Family Welfare Programme – Environment and human health. Human rights – HIV/AIDS – Women and Child Welfare – Role of Information Technology in environment and human health – Disaster management: Floods, earthquake, cyclone and landslides – Case Studies – Activity: Small projects related to environment problems – Social issues and eco friendly technology.

### **Text Books**

1. Raman Shivakumar, "Introduction Environmental science and Engineering", Tata Mc Graw Hill, 2010.
2. Bharucha Erach, "Text book on environmental studies" For Undergraduate Courses of all Branches of Higher Education, University Grants Commission, New Delhi, 2004.
3. Abnubha Kaushik, Kaushik C.P., "Perspectives in Environmental Studies" New Age International Publishers, Third Edition, 2009.
4. Sharma B.K. "Environmental Chemistry" Comprehensive covering the UGC Syllabus, 11th Edition, Goel Publishing House, Meerut, Eleventh Edition, 2007.

### **Reference Books**

1. Trivedi. R.K. "Handbook of Environmental Laws, Rules, Guidelines, Compliances and Standards" Vol. I and II, Enviro Media.
2. Cunningham, Cooper.C.P. and Gorhani, T.H. "Environmental Encyclopedia" Jaico Publ. House, Mumbai, 2001.
3. Gilbert M.Masters, "Introduction to Environmental Engineering and Science" Pearson Education Pvt., Ltd., Second Edition, 2004.
4. T.G. Miller Jr., "Environmental Science", 10th Edition, 2004.
5. Singh. H.R. and Neeraj Kumar. "Ecology and Environmental Science" Vis. Jalandhar 2004.
6. Kidwai.M, Ahluwalia. V. K. "New Trends in Green Chemistry", Kluwer Academic Publishers, 2004.
7. Gerard Kiely, "Environmental Engineering", Tata Mc Graw Hill Pvt. Ltd, 2009.

## **12CH204 PHYSICAL CHEMISTRY**

**Credits: 4:0:0**

### **Course Objective:**

- The speed of a reaction and the criteria for reactions to take place will be discussed.
- The thermodynamic requirement for a chemical reaction to take place and the criteria for spontaneity and reversibility are to be discusses.
- The energy of molecules and quantum chemical explanation given to physical and chemical phenomena will be explained.

### **Course Outcome:**

- The students will explain chemical reactions on the basis of energetic considerations.

### **Unit I**

**THERMODYNAMICS:** Introduction – Zeroth law of thermodynamics – First law of thermodynamics – Internal energy – State functions - Heat Capacities - Relation between  $C_p$  and  $C_v$  (for ideal gases) - Enthalpy – enthalpies of physical and chemical changes – Limitation of first law of thermodynamics – Second law of thermodynamics – Entropy & its significance – Helmholtz Free energy – Gibbs Free energy –Variation of Free energy with temperature and pressure – Third law of thermodynamics.

## Unit II

**CHEMICAL KINETICS AND CATALYSIS:** Introduction – Factors influencing rate of reaction – Order and molecularity of reactions – First order – Second order – Zero order – and pseudo-first order reactions – Half life period – Concept of Activation Energy – Arrhenius theory – Theories of reaction rates: Simple collision theory for bimolecular gaseous reactions – Complex reactions – Definitions of opposing, parallel and consecutive reactions – Catalysis characteristics – Types of catalysis (definition only).

## Unit III

**ELECTROCHEMISTRY:** Redox reactions – Electrode potential – Measurement of electrode potential – Nernst equation for electrode potential – Electrochemical Series & its significance – Types of electrodes – Electrochemical cell or Voltaic cell – Reference electrodes – Hydrogen electrode – Types of Electrochemical cells – Chemical cell & Concentration cell with an example – Batteries - Primary Cell – LeClanche cell - Secondary batteries – Lead acid batteries – Fuel Cell – H<sub>2</sub> – O<sub>2</sub> Fuel cell & its applications.

## Unit IV

**SURFACE CHEMISTRY & COLLOIDS:** Adsorption – Difference between adsorption and absorption – Classification of adsorption – Physisorption – Chemisorption – Adsorption isotherm – Freundlich's adsorption isotherm – Applications of adsorption – Types of solutions – Types of colloidal solutions – Preparation of colloidal solutions – Condensation methods – Disintegrator methods – Purification of colloidal solutions – Dialysis – Ultrafiltration – Characteristics of colloidal solutions – Emulsions – Micelles.

## Unit V

**QUANTUM CHEMISTRY:** Black body radiation – Photoelectric effect – Failure of classical mechanics – Uncertainty principle – Schrodinger wave equation – Eigen functions – Eigen values – Schrodinger equation for hydrogen atom - Particle in one dimensional box.

### Text Books

1. Puri and Sharma, "Principles of Physical Chemistry", Vishal Publishing Co, Jalandhar, 2002.
2. Jain & Jain, "Engineering Chemistry", Dhanpat Rai Publishing Co, New Delhi, 2008.
3. Prasad R.K. "Quantum Chemistry", New Age International Pvt. Ltd., New Delhi, 2002.

### Reference Books

1. Atkins P.W., "Physical Chemistry", Oxford University Press, 8th edition, 2006.
2. Chandra, A.K. "Quantum Chemistry" Tata McGraw – Hill Pvt. Ltd., New Delhi, 4th Edition, 2002.
3. Laidler K.J., "Chemical Kinetics", Harper and Row, New York, 3rd Edition, 2008.
4. Samuel Glasstone, "An Introduction to Electrochemistry", Maurice Press, 2007.

## 12CH205 PRINCIPLES OF ORGANIC CHEMISTRY

**Credits: 3:0:0**

### Course Objective:

- The student will get rudimentary ideas on chemical structure and formula of organic molecules.

- The student will understand the influence of stereoisomerism and conformation in chemical structure and properties of molecules.
- The student will be exposed to ideas about natural products, their structure, and function.

#### **Course Outcome:**

- The students will get knowledge on the structural basics of organic compounds.

#### **Unit I**

**INTRODUCTION TO ORGANIC CHEMISTRY:** Classification of organic compounds – Functional groups – Nomenclature of Organic compounds – Nomenclature of heterocyclic compounds – Fission of bonds – Electrophiles and nucleophiles (Definition, Discussion on the conditions these are formed) – Carbocation and Carbanion, Free radicals, Arynes (Structure and reaction only; methods to identify these species are not required).

#### **Unit II**

**ELECTRONIC EFFECTS AND TYPES OF REACTIONS:** Inductive effect and field effect – Electron delocalization and resonance, Rules of resonance – Steric inhibition of resonance and steric enhancement of resonance (with only one example for each) – Hyperconjugation – Tautomerism - Types of reactions: Substitution reactions (types and examples), Addition reactions (types and examples), Elimination reactions (types and examples), Rearrangement reactions (types and examples) – Thermodynamic and kinetic requirements of a reaction – Kinetic and thermodynamic control – The Hammond postulate.

#### **Unit III**

**STEREOCHEMISTRY I:** Stereoisomerism – Cis-trans isomerism (Definition and examples only) – E, Z nomenclature (Rules and examples only) – Optical isomerism – Cause of optical activity – Racemization – Resolution methods – Absolute configuration – R, S nomenclature – Cahn, Ingold, Prelog nomenclature - Atropisomerism (Biphenyls only) – Asymmetric synthesis - Difference between conformation and configuration – Conformation of ethane, substituted ethanes – Conformation of cyclohexanes, mono, and di-substituted cyclohexanes – Saw-horse, Staggered, Skew, Gauche forms.

#### **Unit 4**

**STEREOCHEMISTRY II:** Dynamic stereochemistry – Stereo-selectivity and stereo-specificity – Curtin-Hammett principle – Enantioselective, Diastereoselective synthesis – Enzymatic and kinetic methods – Effect of conformation on reactivity in acyclic compounds and cyclohexanes.

#### **Unit 5**

**NATURAL PRODUCTS:** Nomenclature, Classification, General methods of structure determination of alkaloids, Terpenoids and flavonoids (Structure determination of any specific natural product is not required)

#### **Text Books**

1. Kalsi. P.S. “Stereochemistry Conformation and Mechanism”, New Age International Publishers, New Delhi, 6th Edition, Reprint, 2005.
2. Mukherji. S. M, and Singh. S.P, “Reaction Mechanism in Organic Chemistry”, Macmillan Publishers, 3rd Edition, Reprinted, 2010.

3. Chatwal Gurdeep. R. "Organic Chemistry of Natural Products, Vol. I & II", Himalaya Publishing House, 5th Revised and Enlarged Edition, New Delhi, 2008.

### Reference Books

1. Jerry March, "Advanced Organic Chemistry", Wiley Eastern Limited, 4th edition, New Delhi, 2008.
2. Finar. I.L., "Organic Chemistry, Volume 1", Doorling Kindersley (Indian), 6th Edition, 5th impression, 2008.
3. Morrison, R.T. & Boyd. R.N. "Organic Chemistry", Pearson Education Pvt Ltd., Singapore, 6th Edition, 2003.
4. Ernest. L. Eliel, "Stereochemistry of carbon compounds", Tata-McGraw Hill, New Delhi, 22nd Reprint, 2009.

## 12CH206 INORGANIC AND COORDINATION CHEMISTRY

**Credits: 4:0:0**

### Course Objective:

- To explain the importance of chemical bonding and acid-base concept.
- To understand the nuclear chemistry.
- To get thorough knowledge about metallurgy of important elements.
- To get thorough knowledge of Transition metal chemistry and their applications in organometallics and bio-inorganic chemistry.

### Course Outcome:

- To apply the various bonding theories and acid-base concept theory.
- To apply the various concepts of transition metal chemistry and their applications in catalysis and bioinorganic chemistry.

### Unit I

**CHEMICAL BONDING:** Types of Bonds – Covalency – VSEPR theory - Valence bond theory and its limitations- Hybridization - MO theory – LCAO method –bond order – MO theory of homo- and heteronuclear diatomic molecules – Comparison between VB and MO theory - Acid-Base concept - Bronsted-Lowry concept - Solvent system – Lewis concept - HSAB concept - Theoretical basis of hardness and softness - Electronegativity and hardness and softness

### Unit II

**NUCLEAR CHEMISTRY:** Properties of nucleus – Nuclear forces – Nuclear stability – Factors affecting nuclear stability – Neutron to proton ratio – Packing fraction – Mass defect – Binding energy – Nuclear reactions – Difference between the chemical reactions and the nuclear reactions – Classification of nuclear reactions – Nuclear fission – Nuclear fusion – Chain reactions – Nuclear reactor – Components of the nuclear reactor

### Unit III

**METALLURGY:** Extraction, Isolation and Purification of some d and f block elements - Titanium, Vanadium, Platinum, Thorium and Uranium – Preparation, Structure and uses of the following compounds -  $\text{TiCl}_4$ ,  $\text{TiO}_2$ ,  $\text{V}_2\text{O}_5$ ,  $\text{H}_2\text{PtCl}_6$ , Thoria, Uranyl Nitrate

#### Unit IV

**TRANSITION METAL CHEMISTRY:** Coordination compound – Polydentate ligands – Isomerism in coordination compounds – Stability of complex compounds in aqueous solution – Thermodynamic stability and kinetic stability – Chelate effect – Theory of metal ligand bonding – VB theory as applied to octahedral, tetrahedral and square planar complexes – Crystal field theory – CFSE -Applications of crystal field theory – MO theory – Sigma bonding only

#### Unit V

**ORGANOMETALLIC CHEMISTRY AND BIOINORGANIC CHEMISTRY:** 18 electron rule – Metal carbonyls – Structure – Metal nitrosyls - Metallocene – Ferrocene – Organometallic compounds in catalysis – Wilkinson’s catalyst – Wacker’s process – Ziegler natta catalysis – Bio-inorganic chemistry (Elementary treatment only) - Metallo-porphyrins – Vitamin B12 – Structure and function – Medicinal inorganic chemistry – Platinum anticancer drugs.

#### Textbooks

1. Satyaprakash, Tuli G. D, Basu S. K & Madan R. D, “Advanced Inorganic Chemistry” Vol I and II, S. Chand and Company Ltd, NewDelhi, India, Reprint 2009.
2. Lee J. D, “Concise Inorganic Chemistry”, Wiley India (P.) Ltd, New Delhi, India, 5th edition, Reprint 2009.

#### Reference Books

1. Cotton F. A. & Wilkinson G, “Advanced Inorganic Chemistry”, Wiley India (P.) Ltd, New Delhi, India, 6th edition, First Reprint 2007.
2. Madan R. D, “Modern Inorganic Chemistry”, S. Chand and Company Ltd, NewDelhi, India, 3rd edition, 2011.

### 12CH207 ORGANIC REACTIONS AND MECHANISMS

**Credits: 4:0:0**

#### Course Objective:

- Chemical reactions, which are mostly used to synthesize compounds of various types, and their mechanism are discussed.
- Distinguishing the types of reactions and their mechanism will give an idea of the structural requirements of reactions of a particular type.
- The student will be able to write a reaction by explaining which bonds are broken and in what order.

#### Course Outcome:

- The student will get a thorough knowledge on reactions of organic compounds and different types of mechanisms which he will use in synthesis of nanoscale materials.
- He will understand how classical chemistry is related to nanochemistry in terms of synthesis.

#### Unit I

**AROMATIC AND ALIPHATIC NUCLEOPHILIC SUBSTITUTIONS:** The  $S_NAr$  mechanism –  $S_N1$  mechanism – Benzyne mechanism – Reactivity – Effect of substrate structure, Leaving group, Attacking nucleophile – Bucherer reaction – Chichibabin reaction –  $S_N1$  and  $S_N2$

mechanisms – Neighboring group participation – Non-classical carbocations – Effect of substrate structure, Attacking nucleophile, Leaving group, and reaction medium on nucleophilic substitution – Ambident nucleophiles and regioselectivity.

### Unit II

**AROMATIC AND ALIPHATIC ELECTROPHILIC SUBSTITUTIONS:** Arenium ion mechanism – Orientation and reactivity in mono-substituted aromatic rings – Quantitative treatment – Hammett equation – Effect of leaving group – Nitration, Diazonium coupling, Nitrosation, – Mechanisms  $S_E2$  mechanism –  $S_E1$  mechanism – Reactivity – Aliphatic diazonium coupling – Acylation at an aliphatic carbon – The Stork-enamine reaction.

### Unit III

**ADDITION AND ELIMINATION REACTIONS:** Addition reactions - Electrophilic, Nucleophilic, and free-radical addition to double and triple bonds – Hydration, Hydroxylation, Michael addition, Hydroboration - Addition to carbonyl compounds – Mannich reaction Elimination reactions – mechanism –  $E_1$ ,  $E_2$  mechanisms, Hofmann, Saytzeff rules, Bredt's rule – Chugaev reaction, Hofmann degradation.

### Unit IV

**COMMON ORGANIC REACTIONS:** Aldol, Perkin, Dieckman condensations – Reimer-Tiemann, Grignard reactions – Gattermann reaction, Friedel-Crafts reaction, Wittig reaction – Functional group transformations and interconversion of simple functionalities – Clemmensen, Wolff-Kishner, Meerwein-Ponndorf-Verley reductions.

### Unit V

**MOLECULAR REARRANGEMENTS:** Baeyer-Villiger rearrangement – Fries, Benzidine and Stevens rearrangements – Benzil-benzilic acid rearrangement – Favorski rearrangement – Curtius, Lossen, Sommelet-Hauser rearrangement – Hoffmann rearrangement.

### Text Books

1. Gurdeep R. Chatwal, "Reaction Mechanism and Reagents in Organic Chemistry", Himalaya Publishing House, New Delhi, 2007.
2. Jerry March, "Advanced Organic Chemistry", Wiley Eastern Limited, 4th edition, New Delhi, 2008.
3. Hassner. A, and Stumer. C, "Organic Synthesis based on name reactions", Pergamon Press, 1st Edition, 2002.

### Reference Books

1. Carey, F.A, and Sundberg. R. J, "Advanced Organic Chemistry Part – B: Reactions and Synthesis", Plenum Press, 2008.
2. Finar. I.L., "Organic Chemistry, Volume 2", 6th Edition, 5th Impression, Doorling Kindersley (Indian), 2008.
3. Mukherji S. M, and Singh. S.P, "Reaction Mechanism in Organic Chemistry", Macmillan Publishers, 3rd Edition, Reprinted, 2010.
4. Ahluwalia, V. K, and Rakesh Kumar Parashar, "Organic Reaction Mechanisms", Narosa Publishing House, New Delhi, 4th Edition, 2011.

## 12CH208 MATERIALS CHEMISTRY

**Credits: 4:0:0**

### **Course Objective:**

- Since atoms are the building blocks of materials and life, the student will learn the theories behind atomic structure.
- The student will learn the types of materials and their bonding features.
- The student will be able to distinguish between the chemical and physical nature of various categories of materials.

### **Course Outcome:**

- The students will get knowledge on the building blocks of materials, the bonding involved, and their function.

### **Unit I**

**ATOMIC STRUCTURE:** Structure of atom – Defects of Rutherford's model - Bohr's model of an atom – Sommerfield's extension of atomic structure – Electronic configuration and quantum numbers – s, p and d orbitals - Pauli's exclusion principle – Hund's rule of maximum multiplicity – Aufbau principle – Ionic radius, Ionization potential, Electron affinity, Electronegativity (Definitions with examples only; trend in group and period not required) – Sigma and pi bonds – Hydrogen bonding – Van der Waals' forces - Bond lengths and bond angles (With reference to single and multiple bonds) – Particles: leptons, quarks, gauge bosons, fermions (Brief discussion on their charge, physical existence only).

### **Unit II**

**SOLID STATE:** Crystal structure – Crystal symmetry – Unit cell – The seven crystal systems – The 14 Bravais lattices – Reciprocal lattice - Defects in crystals – Point defects, Line defects, Planar defects – Dislocations – Edge dislocations, Screw dislocations – Slip and plasticity.

### **Unit III**

**METALS:** Metallic bonding – Ductility and conductivity – Alloys – Classification as base metals, Ferrous metals, Noble metals and precious metal – Structure of metals: 12 coordination, 8 coordination, Crystal grains – Properties of metals – Thermal spray, Case hardening, Plating – Metal testing: nondestructive testing – Metallography.

### **Unit IV**

**POLYMERS:** Classification of polymers – Polymer morphology: Crystallinity, Tensile strength, Young's modulus – Phase behavior: Glass transition temperature, Mixing behavior, Inclusion of plasticizers – Types of polymerization – Mechanisms – Important polymers (Preparations and uses only): Polyethylene, Polyvinyl chloride, Bakelite, Rubber, Silicones – Polymer degradation.

### **Unit V**

**CERAMICS AND COMPOSITES:** Ceramics - introduction – Types of ceramic products – Types of ceramic materials: Crystalline and non-crystalline – Properties ceramics: Mechanical, Electrical, and Optical properties – Applications. Composites: introduction – Moulding methods – Properties composites: Mechanics, resins – Polymer composites – Fiber glass – Fiber reinforced plastic – Uses

### **Text books**

1. Brian S. Mitchell, "An Introduction to Materials Engineering and Science for Chemical and Material Engineers", Wiley Inter-science, 2004.
2. William D. Callister, "Fundamentals of Materials Science and Engineering", Ed. 5, John Wiley & sons, 2001.

### **Reference books**

1. Robert E. Newnham, "Properties of Materials", Oxford university press, 2005.
2. Deborah D.L. Chung, "Applied Materials Science", CRC Press, Chapman and Hall, 2001.
3. Wole Soboyejo, "Mechanical Properties of Engineered Materials", Marcel Dekker Inc., 2002.

## **12CH209 BIOCHEMISTRY**

**Credits: 3:0:0**

### **Course Objective:**

- The student will get ideas on biomolecular structure and their functional role.
- The student will understand the influence of biomolecules in bodily processes.
- The student will be exposed to ideas about separation and classification of large molecules.

### **Course Outcome:**

- The students will get knowledge about the structure, properties, and action of biomolecules.

### **Unit I**

**PROTEINS AND NUCLEIC ACIDS:** Amino acids and proteins: Definition, General Properties – Primary, Secondary, Tertiary, Quaternary and 3-D Structures of Proteins - Chemical Synthesis of Poly peptides. Nucleic acids: Definition, composition, structures of purines, pyrimidines, Phosphodiester bonds and Sugars - Classification of Nucleic acids, Differences between DNA and RNA - Solid Phase synthesis of DNA (Sanger's method) Separation and Purification of Amino acids and Proteins: Paper, Gel Filtration Chromatography, Gel Electrophoresis, Western blotting.

### **Unit II**

**CARBOHYDRATES AND LIPIDS:** Carbohydrate – Definition, classification, conformation of furanose and pyranose rings, general Properties – glycoproteins, proteoglycans: Structure and functions - Fatty acids: Structure, and function - Membrane lipids: classification as phospholipids, sulfolipids, spingolipids and glycolipids, their importance - lipoproteins, diffusion of proteins into the plane of membrane proteins.

### **Unit III**

**ENZYMES: MECHANISM AND KINETICS:** Enzymes – definition, IUB classification, nomenclature - Enzymes as specific catalyst, Lock & key and induced fit theories, Inhibitors for enzyme reactions - Free energy and transition state changes - Michaelis-Menten and Lineweaver-Burk plot - Proteases: facilitators of specific reactions, Protease inhibitors as drugs - Hemoglobin–oxygen binding.

#### **Unit IV**

**METABOLISM AND BIOENERGETICS:** Metabolism – definition, coupled and interconnecting reactions - Metabolic pathways with recurring motifs - Cellular energy: Oxidation of carbon fuels - Role of hormones and signal transduction in the metabolic pathways.

#### **Unit V**

**RECEPTORS AND METABOLISM:** Trans-membrane and intracellular receptors - calcium as ubiquitous cytosolic messenger - Glycolysis, HMP-shunt pathway, glycogenesis, glycogenolysis, gluconeogenesis, TCA cycle and mitochondrial Electron transport chain - An overview of amino acid metabolism.

#### **Text Books**

1. Basic concepts in biochemistry, H.F. Gilbert, McGraw Hill, Ed. 2, 2002
2. Lehninger, Principles of biochemistry, David L. Nelson, Michael M. Cox, Ed. 4, 2002

#### **Reference Books**

1. Biochemistry, J.M. Berg, J.L. Tymoczko, L. Stryer, Ed. 5, W.H. Freeman & Co., 2004
2. Biochemistry notes, Lynne B. Jorde, Kaplan Inc., 2002
3. Biochemistry, G. N. Wilson, McGraw Hill co., 2002

## **12CH210 CHARACTERIZATION AND INSTRUMENTAL TECHNIQUES**

**Credits: 4:0:0**

#### **Course Objective:**

- Since nanotechnology had its origin on the technological advancements of probing structures a study in combination of classical and modern techniques is required.
- The student will understand the ways of identifying molecules and materials based on spectral and microscopic techniques.
- The student will be able to distinguish between light scattering, absorption, and emission spectral techniques and those do not involve light sources.

#### **Course Outcome:**

- The students will get knowledge on analyzing the structure of molecules and materials.

#### **Unit I**

**MICROSCOPY & XRD:** Scanning electron microscopy (SEM) – scanning tunneling microscopy (STM) – transmission electron microscopy (TEM) – X-ray diffraction (XRD) – extended X-ray absorption fine structure (EXAFS) (physical principles and instrumentation only to be discussed for all the techniques).

#### **Unit II**

**DIFFRACTION AND SCATTERING TECHNIQUES:** Neutron diffraction – low energy electron diffraction (LEED) – reflection high energy electron diffraction (RHEED) – electron energy loss spectroscopy (EELS) - reflected electron energy loss spectroscopy (REELS) -

Dynamic light scattering (DLS) (physical principles and instrumentation only to be discussed for all the techniques).

### Unit III

**VIBRATIONAL SPECTROSCOPY:** Introduction to spectroscopy – spectroscopic regions and classifications - the vibrating diatomic molecule – vibrational transitions - selection rule – simple harmonic oscillator – anharmonic oscillator – the diatomic rotor – vibrations of polyatomic molecule – factors influencing vibrational frequencies – identification of functional groups – finger print region – application to organic compounds – instrumentation.

### Unit IV

**ULTRAVIOLET AND VISIBLE SPECTROSCOPY:** Electronic spectra of diatomic molecules – physical principles – laws of absorption – absorption transitions – chromophores and auxochromes – effects of conjugation – Woodward-Fieser rules for  $\alpha,\beta$ -unsaturated carbonyl compounds and dienes – aromatic systems with extended conjugation – application to organic and inorganic compounds – instrumentation.

### Unit V

**NANOTRIBOLOGY, PHOTOELECTRON SPECTROSCOPY:** Nanotribology – nanotribometer – surface force apparatus – quartz crystal microbalance – friction force microscope – X-ray photoelectron spectroscopy (XPS) – electron spectroscopy for chemical analysis (ESCA) – ultraviolet photoelectron spectroscopy (UPS) (physical principles and instrumentation only to be discussed for all the techniques).

### Text Books

1. The chemistry of nanomaterials, C.N.R. Rao, A. Muller, A.K. Cheetham, Wiley VCH, 2004.
2. Introduction to Nanotechnology, Charles P Poole Jr., and Frank J. Ownes, John Wiley Sons, Inc., 2003.
3. Colin N. Banwell & Elaine M. McCash, Fundamentals of Molecular Spectroscopy, 4<sup>th</sup> Edition, McGraw-Hill, New Delhi, 2004.

### Reference Books

1. Synthesis, Functional Properties and Applications of Nanostructures, T. Tsakalakos, I. Ovid'ko and A.K. Vasudevan (eds.), Kluwer Academic Publishers, Dordrecht, 2003.
2. Instrumental methods of Analysis, H.A. Willard and L.L. Merrit, J.A. Dean, Van Nostrand, New York, 1986.
3. Nano: The Essentials, T. Pradeep, Tata McGraw Hill, New Delhi, 2007.
4. Jag Mohan, Organic Spectroscopy Principles and Applications, Narosa Publishing House, New Delhi, 2001.
5. D.N. Satyanarayana, Vibrational Spectroscopy Theory and Applications, New Age International Publishers, New Delhi, 2004.

## 12CH211 MEDICINAL CHEMISTRY

**Credits: 4:0:0**

### **Course Objective:**

- The student will use his earlier knowledge on organic structures to design a drug.
- The student will understand the mechanism of drug action and various phases of drug development.
- The student will be exposed to ideas about target-based drug design and clinical trial of drugs.

### **Course Outcome:**

- A thorough idea of drug chemistry and the structure–action relationship will be given.

### **Unit I**

**BASICS OF MEDICINAL CHEMISTRY:** Brief history of medicinal chemistry – classification of drugs – brief description of biological, chemical, computer revolutions in drug design – pro drugs and soft drugs – design of pro drug system – multiple pro drug formation – soft drug principle and applications.

### **Unit II**

**DRUG TARGETS AND DRUG SOLUBILITY:** Enzymes and enzyme inhibitors – competitive and non-competitive inhibitors – reversible and irreversible inhibitors – ligand-receptor theories – Clark's theory and Paton's rate theory – proteins, lipids, and nucleic acids as drug targets – effect of pH,  $pK_a$ , and polarity on drug solubility.

### **Unit III**

**PHARMACOKINETICS AND DRUG METABOLISM:** Natural resources of lead compounds – absorption, distribution, metabolism, and elimination – oxidation and hydrolysis – testing drugs in vitro – high-throughput screening – testing drugs in vivo – therapeutic index and therapeutic ratio.

### **Unit IV**

**CLINICAL TESTING AND SYNTHESIS OF DRUGS:** Various phases in preclinical testing and clinical trials – designing organic synthesis – convergent synthesis – patenting and manufacture – complexes and chelating agents – metal clusters – detoxification – drug action and metal chelation.

### **Unit V**

**DEVELOPMENT OF NEW DRUGS:** Five classic steps in the design of a new drug – procedures in drug design – isolation of bioactive compounds – accidental discovery – examination of metabolites – interference with fundamental life processes – exploitation of side effects of drugs - random screening – synthesis of drugs ab initio – molecular modification of lead compounds – factors affecting drug development.

### **Text Books**

1. Foye's Principles of Medicinal Chemistry, 5th edition; David A. Williams, William O. Foye, Thomas L. Lemke; Lippincott Williams & Wilkins: Philadelphia, 2002.

2. Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry, 11th edition; Delgado & Remers, Eds.; Lippincott Williams & Wilkins: Philadelphia, 2004 ("W&G").

### Reference Books

1. Burger's Medicinal Chemistry, 6th ed., Vol. 1-6; D.J. Abraham, Ed. (RS403 .B8 2003 - vol.1-6).
2. Organic Chemistry of Drug Synthesis, Vol. I-6, Daniel Lednicer and Lester, A. Mitscher (RS 403.L38-vol. 1-6).
3. Goodman & Gilman's the Pharmacological Basis of Therapeutics, 10th ed., Joel G. Hardman & Lee L. Limbird, Eds.; Alfred Gilman, Contrib. Ed (RM300 .G644 2001).

## 12CH212 ANALYTICAL CHEMISTRY AND SPECTROSCOPY

**Credits: 4:0:0**

### Course Objective:

- The separation methods of compounds and their purification will be discussed.
- The student will understand the structure analysis using spectral techniques.
- The student will distinguish between the principles of techniques which are used to study solution phase samples and to study solid samples.

### Course Outcome:

- The students will know separation and structure analysis of molecules and materials.

### Unit I

**ANALYTICAL TECHNIQUES:** Chromatography: theory, instrumentation, basic principles and applications of the following – Column, thin layer, and ion-exchange chromatography – HPLC - applications in chemical analysis – Gas chromatography - Principles of ORD and CD – Cotton effect – Octant rule – Axial haloketone rule – Applications of ORD and CD in organic and bio-molecules.

### Unit II

**NMR SPECTROSCOPY:** Principle of NMR spectroscopy – Instrumentation – Factors affecting chemical shifts – Chemical and magnetic equivalence – Proton NMR – Spin-spin coupling – FT NMR –  $C^{13}$  NMR – Factors affecting chemical shifts – Application of NMR to structure determination of organic compounds – Decoupling – Off-resonance decoupling.

### Unit III

**EMISSION SPECTROSCOPY:** Photoluminescence – Fluorescence and phosphorescence – Jablonskii diagram – Fluorescence polarization – Fluorescence correlation spectroscopy (FCS) – Fluorescence in-situ hybridization (FISH) – Fluorescence confocal microscopy – Fluorescence resonance energy transfer (FRET) - (physical principles, instrumentation and applications).

### Unit IV

**MASS SPECTROMETRY:** Principles of mass spectrometry – Nitrogen rule – Meta-stable ions and peaks – Molecular ion peak – Fragmentation processes – Even and odd electron ions – Retro-Diels-Alder rearrangement – McLafferty rearrangement – Fragmentation associated with

functional groups – Aldehydes and ketones, carboxylic acids, esters, amides and alcohols, thiols and amines, aromatic compounds.

### Unit V

**INTRODUCTION TO CRYSTALLOGRAPHY:** Introduction to X-ray crystallography – Protein crystallography – Problems associated with growing biomolecular crystals – Isomorphous replacement in solving crystal structure – Interpretation of derived electron density maps – Land mark modules in crystallography (physical principles and instrumentation only to be discussed for all the techniques).

### Text Books

1. Ewing, G.W. Instrumental Methods of Chemical Analysis, 5th Edition, 1978, McGraw Hill Books Co., New York.
2. Kalsi, P.S. Spectroscopy Of Organic Compounds, 6th Edition, New Age International Publishers, New Delhi, 2004.
3. Sharma, Y.R. Elements Of Organic Spectroscopy, S. Chand & Company Ltd., New Delhi, 2004.

### Reference Books

1. Skoog, D.A. Principles of Instrumental Analysis, 5th Edition, 1998, Saunders College Publishing, Philadelphia, London.
2. Kennedy, J.H. Analytical Chemistry: Principles, 2nd Edition, 1990, Saunders Holt, London.
3. Robert M. Silverstein & Francis X. Webster, Spectroscopy of Organic Compounds, 6th Edition, Wiley Publications, 1998
4. Straughan B.P. & Walker, S. Spectroscopy, John Wiley and Sons, New York (1976).
5. Introduction to solid state physics, Charles Kittel, John Wiley and sons, 1953.

## 12CH213 SUPRAMOLECULAR CHEMISTRY

**Credits: 4:0:0**

### Course Objective:

- As the students have known the structural and functional basics of building blocks of supramolecular structures, he/she will now be taught how to build up such structures.
- A knowledge on the driving forces of supramolecular structure formation will be given to the student.
- The student will be exposed to ideas on the types of supramolecules based on structure and the chemistry behind host-guest assembly.

### Course Outcome:

- The structure of supramolecules of various types in solution and solid state and their importance as materials and functional units will be learnt by the student.

### Unit I

**INTRODUCTION TO SUPRAMOLECULAR CHEMISTRY:** Introduction to supramolecular chemistry – Selectivity – Lock and key principle and induced fit model – complementarity – Co-operativity and chelate effect – Pre-organization – Binding constants – Kinetic and thermodynamic selectivity – Optically active supra-molecules – Self-assembly of

intrinsically chiral molecular capsules – Chiral induction in the formation of supra-molecular systems – Chiral memory effect – Chiral nanoparticles.

### Unit II

**SOLUTION HOST–GUEST CHEMISTRY:** Introduction: guests in solution – Macrocyclic vs. acyclic hosts – High-dilution synthesis – Template synthesis – Cation binding – Crown ethers and cryptands – Spherands – Heterocrowns – Biological ligands: ion channels – Anion binding – Charged receptors – Neutral receptors – Lewis acid receptors – Neutral molecule binding – Calixarenes, cyclodextrins and dendrimers as catalysts.

### Unit III

**SUPRAMOLECULAR STRUCTURES:** Ladders, polygons, and helices – Self-assembly using metal templates – Racks, ladders, and grids – Helicates – Molecular polygons – Rotaxanes, catenanes, and knots – Topological connectivity – Rotaxanes and catenanes as molecular devices – Borromeates – Knots (structure and function of the above species).

### Unit IV

**SOLID STATE SUPRAMOLECULAR CHEMISTRY:** Introduction – Zeolites: structure – Zeolite composition – Zeolites and catalysis – Clathrates – Urea/thiourea clathrates – Trimesic acid clathrates – Hydroquinone and Dianin's compound – Clathrate hydrates (structure and function of the above species) – Uses.

### Unit V

**SELF-ASSEMBLING CAPSULES:** Self-assembling capsules – Molecular containers – Metal directed capsules – Hydrogen bonded capsules – Concepts in crystal engineering – The Cambridge structural database - Crystal engineering with hydrogen bonds – Pi interactions - Solid state reactivity – Metal-organic frameworks – Guest properties of metal-organic frameworks.

### Text books

1. Jean-Marie Lehn, Supramolecular Chemistry, RCS pubs., 2005.
2. Jonathan Steed, David Turner, Carl Wallace, Core concepts in Supramolecular Chemistry and nanochemistry, John Wiley & sons, 2007.
3. Supramolecular chemistry – Fundamentals and applications advanced textbook, Katsuhiko Ariga · Toyoki Kunitake, Springer-Verlag, 2000.

### References

1. <http://www.uaf.edu/chem/rfk/nano.htm>
2. Nano: The essentials, T. Pradeep, McGraw Hill Publishers, 2007.
3. Nanochemistry, G.B. Sergeev, Elsevier, 2007.
4. Nanomaterials and nanochemistry, C. Brechignac, P. Houdy, M. Lahmani, Springer, 2006.

## 12CH214 CHEMINFORMATICS

**Credits: 4:0:0**

### Course Objective:

- The learnt concepts of structure, medicinal properties of chemical species will be applied in describing them using computer.

- The graphical way of representation of chemical structures will be discussed
- Choosing the best structure for drug design will be taught.

#### **Course Outcome:**

- The students gain knowledge on virtual screening methods in structure searching and design.

#### **Unit I**

**REPRESENTATION OF 2D MOLECULAR STRUCTURES:** Cheminformatics: definition and scope – Use of cheminformatics – Evolution of cheminformatics – Computer representation of chemical structures – Graph theoretic representation of chemical structures – Connection tables and linear notions – Canonical representations of molecular structures – Structure searching, substructure searching – Screening methods – Reaction databases.

#### **Unit II**

**REPRESENTATION OF 3D MOLECULAR STRUCTURES:** Introduction to 3D representation – experimental 3D databases – 3D pharmacophores – Theoretical 3D databases: structure generation programs, conformational search and analysis – Random conformational search – Methods to derive 3D pharmacophores, pharmacophore mapping using constrained systematic search – Pharmacophore mapping using clique detection, maximum likelihood method for pharmacophore mapping – Practical aspects of pharmacophore mapping – Applications of 3D pharmacophore mapping.

#### **Unit III**

**MOLECULAR DESCRIPTORS:** Introduction – Descriptors calculated from 2D structure: simple counts, physicochemical properties, molar refractivity – Topological indices, kappa shape indices – Electro-topological state indices – 2D finger prints – Descriptors based on 3D representations – 3D fragment screens, pharmacophore keys – Data verification and manipulation: data spread and distribution, scaling – correlations between descriptors – Principal component analysis – Reducing the dimensionality of a data set.

#### **Unit IV**

**SIMILARITY METHODS:** Introduction – Similarity based on 2D finger prints – Similarity coefficients – Other 2D descriptor methods (Maximum common sub graph similarity) – 3D similarity – Alignment independent methods – Alignment methods: field based alignment – Gnomonic projection methods – Finding the optimal alignment – Comparison and evaluation of similarity methods.

#### **Unit V**

**ANALYSIS OF HIGH-THROUGHPUT SCREENING DATA; VIRTUAL SCREENING:** Introduction – Data visualization – Non linear mapping – Data mining methods; sub structure analysis – Discriminant analysis – Neural networks – Decision trees – Introduction to virtual screening – Drug likeness and compound filters – Structure based virtual screening; protein-ligand docking – Scoring functions for protein- Ligand docking.

#### **Text Books**

1. Andrew R. Leach, Valerie J. Gillet, An introduction to chemoinformatics, Springer, 2005.

- Richard G. Brereton, Chemometrics Data Analysis for the Laboratory and Chemical Plant, John Wiley & sons, 2003.

### Reference books

- Johann Gasteiger, Thomas Engel, Chemoinformatics, Wiley-VCH, 2003.
- Jure Zupan, Johann Gasteiger Neural networks in chemistry and drug design, , Wiley-VCH, 1999.
- H. Holtje, W. Sippl, D. Rognan, G. Folker, Molecular modeling, Wiley-VCH, 2003.
- B.A. Bunin, J. Bajorath, B. Siesel, G. Morales, Chemoinformatics: theory, practice, and products, Springer, 2007.

## 12CH215 QUALITATIVE ANALYSIS AND INORGANIC PREPARATIONS LAB

**Credits: 0:0:2**

### Course Objective:

- To provide the students an appreciation for the synthesis of Inorganic Complexes.
- To provide the students a competence in the laboratory skills required for accurate and precise chemical analysis.
- The students will know the theoretical basis of qualitative inorganic analysis containing common and less common ions.

### Course Outcome:

- The student will gain the laboratory skills to synthesize the inorganic complexes, to estimate the amount of metals quantitatively by complexometric and redox titrations and will be confident in analyzing the mixtures containing common and less common ions using semimicro analysis.

### QUALITATIVE ANALYSIS AND INORGANIC PREPARATIONS:

- Analysis of mixtures containing one anion and one cation from the following:  
Anions: Carbonate, sulfide, sulphate, chloride, bromide, iodide, acetate, nitrate, oxalate, tartrate, borate, phosphate, arsenate and chromate.  
Cations: Lead, copper, bismuth, cadmium, tin, antimony, iron, aluminum, zinc, manganese, nickel, cobalt, calcium, strontium, barium, potassium and ammonium.

Preparations: Any three of the following inorganic preparations:

- Ferrous ammonium sulphate
- Tetrammine copper (II) sulphate
- Potassium trisoxalato chromate (III)
- Potash alum  $KAl(SO_4)_2 \cdot 2H_2O$
- Hexammine cobalt (III) chloride
- Manganous sulphate
- Microcosmic salt
- Sodium thiosulphate

12 experiments will be notified by HOD from time to time

### Reference Books

1. Jeffery, G.H. Bassett, J. Mendham J. and R.C. Denney, "Vogel's text book of quantitative chemical analysis", ELBS, 5th Edn. Longman, Singapore publishers, Singapore, 1996
2. Kolthoff I.M. and Sandell, E.B. "Quantitative Chemical Analysis" MacMillan, Chennai, 1980
3. Svehla, G. "Vogel's Qualitative Inorganic Analysis", 6th Edn., Orient Longman, New Delhi, 1987
4. Ramanujan, V. "Inorganic Semi-micro Qualitative Analysis", 3rd Edn., National Publishing Company, Chennai, 1990.
5. Manivasakam, K. "Physico-chemical Examination of Water Sewage and Industrial Effluents", 3rd Edn., Pragati Prakashan, Meerut, 1996.

## 12CH216 ORGANIC QUALITATIVE ANALYSIS LAB

**Credits: 0:0:2**

### Course Objective:

- To enrich the knowledge of Organic Laboratory skills for single step preparation, estimation and analysis of Organic mixture.

### Course Outcome:

- Students acquire the knowledge of synthesis, estimation and analysis of Organic Compounds.

### ORGANIC QUALITATIVE ANALYSIS:

- Identification of an organic compound through the functional group analysis, determination of melting point and preparation of suitable derivatives. [Detection of elements (N, S and halogens) and functional groups (phenolic, carboxylic, carbonyl, esters, carbohydrates, amines, amides, nitro and aniline) in simple organic compounds].
- Separation of two component mixtures - 1) Aniline + Naphthalene 2) Benzoic acid + Benzophenone 3) p-Cresol + Chlorobenzene.

12 experiments will be notified by HOD from time to time

### Reference Books

1. Vogel A.I. – "Text book of practical organic chemistry", 5th Ed. ELBS, London, 1989.
2. Dey B.B. and Sitharaman M.V., "Laboratory manual of Organic Chemistry" Revised by T.R. Govindachari, Allied Publishers Ltd., New Delhi, 4th Revised edition, 1992.
3. Palleros, Daniel R. "Experimental Organic Chemistry" John Wiley & Sons, Inc., New York, 2000.
4. Fumiss B.S, Hannaford A.J, Rogers V, Smith P.W.G. and Tatchell A.R., "Text book of Practical Organic Chemistry", LBS, Singapore, 1994.
5. Khopar S.M., "Basic concepts of Analytical Chemistry", John Wiley & Sons, 1984.

## 12CH217 TITRIMETRIC ANALYSIS AND GRAVIMETRIC ANALYSIS LAB

**Credits: 0:0:2**

### **Course Objective:**

- To enrich the knowledge of estimation through titrimetric and gravimetric skills

### **Course Outcome:**

- Students acquire the knowledge of acidimetry, permanganometry, iodometry, complexometry, dichrometry and gravimetry.

### **I. TITRIMETRIC ANALYSIS:**

#### **ACIDIMETRY**

- Estimation of sodium hydroxide – standard sodium carbonate.
- Estimation of borax – standard sodium carbonate
- Estimation of bicarbonate and carbonate in a mixture

#### **PERMANGANOMETRY**

- Estimation of oxalic acid - standard - Mohrs salt or ferrous sulphate
- Estimation of calcium
- Estimation of sodium nitrite - standard - Oxalic acid
- Estimation of ferric ion
- Estimation of percentage of manganese in pyrolusite

#### **IODOMETRY**

- Estimation of arsenious oxide
- Estimation of copper – standard potassium dichromate
- Estimation of potassium dichromate – standard copper sulphate

#### **COMPLEXOMETRY**

- Estimation of zinc or magnesium using EDTA
- Estimation of zinc using potassium ferrocyanide
- Estimation of temporary and permanent hardness of water

#### **DICHROMETRY**

- Estimation of ferrous ion using diphenylamine I N-.Phenyl anthramlic acid as indicator.
- Precipitation titration - Estimation of chloride in neutral medium

## II. GRAVIMETRIC ANALYSIS

- Determination of barium as barium sulphate
- Determination of sulphate as barium sulphate
- Determination of lead as lead chromate
- Determination of nickel as Ni-DMG complex
- Determination of magnesium as magnesium pyrophosphate.

12 experiments will be notified by HOD from time to time

### Reference Books

1. Jeffery, G.H. Bassett J., Mendham J. and Denney R.C., "Vogel's text book of quantitative chemical analysis", ELBS, 5th Edn. Longman, Singapore publishers, Singapore, 1996.
2. Kolthoff I.M. and Sandell E.B., "Quantitative Chemical Analysis" MacMillan, Chennai, 1980.
3. Svehla G., "Vogel's Qualitative Inorganic Analysis", 6th Edn., Orient Longman, New Delhi, 1987.
4. Ramanujan V., "Inorganic Semi-micro Qualitative Analysis", 3rd Edn., National Publishing Company, Chennai, 1990.
5. Manivasakam K., "Physico-chemical Examination of Water Sewage and Industrial Effluents", 3<sup>rd</sup> Edn., Pragati Prakashan, Meerut, 1996.

## 12CH218 PHYSICAL CHEMISTRY LAB

Credits: 0:0:2

### Course Objective:

- To carryout simple chemical reaction which would be monitored by Electrical and Non - Electrical experimental studies.

### Course Outcome:

- The analytical skill will be improved by pursuing electrical experiments like Conductometry, Spectrophotometry, Potentiometry.
- The basic knowledge could be understood thoroughly regarding the velocity of the reaction, distribution properties and adsorption studies.

### CHEMICAL KINETICS

- Determination of specific reaction rate of the hydrolysis of methyl acetate catalyzed by hydrogen ion at room temperature.
- Determination of rate of decomposition of hydrogen peroxide.
- Determination of overall order of saponification of ethyl acetate.

### DISTRIBUTION LAW

- Determination of distribution coefficient of iodine between water and carbon Tetrachloride.
- Determination of molecular status and partition coefficient of benzoic acid in Toluene and water.

## **ELECTROCHEMISTRY**

- Determination of concentration of HCl conductometrically using standard NaOH solution.
- Determination of concentration of acetic acid conductometrically using standard NaOH solution.
- Determination of dissociation constant ( $K_a$ ) of acetic acid by conductivity measurements.
- Determination of solubility and solubility product of  $BaSO_4$
- Determination of redox potentials of  $Fe^{2+}/Fe^{3+}$  by potentiometric titration of ferrous ammonium sulphate vs. potassium dichromate.

## **pH METRY**

- Preparation phosphate buffer solutions.
- pH metric titration of weak acid, acetic acid with strong base NaOH and calculation of dissociation constant.

## **COLORIMETRY**

- Verification of Beer-Lambert law for  $KMnO_4$ ,  $K_2Cr_2O_7$  and determination of concentration of the given solution.
- Verification of Beer-Lambert law for  $CuSO_4$  and determination of concentration of the given solution.
- Composition of complex of  $Cu^{2+}$  - EDTA disodium salt

## **ADSORPTION**

- Surface tension and viscosity of liquids.
- Adsorption of acetic acid on animal charcoal, verification of Freundlich isotherm.

12 experiments will be notified by HOD from time to time

## **Reference Books**

1. Willard – Dean – Merrit, “Instrumental methods of analysis”, Affiliated East West pvt. Ltd., New Delhi, 1965.
2. Vogel A.I. – “Text book of quantitative inorganic analysis”, Long man group Ltd., 1978.
3. Shoemaker, D.P, Garland, C.W, Nibbler J.W. “Experiments in Physical Chemistry” McGraw Hill 5th Edition, 1989.
4. Khosala B.D, Gulnti A. and Garg V.C., “Senior practical physical chemistry” 7th edition, S. Chand & Co., New Delhi, 1994.
5. Satiya D.R., ‘Practical Chemistry’, 2nd edition, Allied publishers Ltd., Chennai, 1991.

## **12CH219 SYNTHESIS OF ORGANIC COMPOUNDS AND CHROMATOGRAPHY LAB**

**Credits: 0:0: 2**

### **Course Objective:**

- To enrich the knowledge of synthesis of Organic compounds and analysis of Organic mixture by chromatography.

**Course Outcome:**

- Students acquire the knowledge of synthesis and separation of Organic Compounds.

**1. Synthesis of Organic Compounds**

- Aromatic electrophilic substitution Nitration: Preparation of nitro benzene and p-nitro acetanilide, Halogenation: Preparation of p-bromo acetanilide – preparation of 2,4,6-tribromo phenol.
- Diazotization and coupling: Preparation of p-phenyl azo  $\beta$ -naphthol
- Oxidation: Preparation of benzoic acid from benzoyl chloride
- Reduction: Preparation of m-nitro aniline from m-dinitro benzene
- Esterification: Preparation of methyl p-nitro benzoate from p-nitro benzoic acid.
- Methylation: Preparation of  $\beta$ -naphthyl methyl ether
- Condensation: Preparation of benzilidene aniline and Benzoyl aniline.

**2. Thin layer Chromatography & Column Chromatography**

- Preparation of the TLC plates. Checking the purity of the compounds by TLC: Acetylation of salicylic acid, aniline, Benzoylation of Aniline and Phenol  
Determination of R<sub>f</sub> values and identification of organic compounds by TLC: preparation and separation of 2,4-dinitrophenyl hydrazones of acetone and 2-butanone using toluene and light petroleum(40:60)
- Separation of ortho & para nitro aniline mixture by column chromatography

**3. Demonstration experiments:**

- Steam distillation experiment: separation of ortho and para nitro phenols 2) Microwave assisted Green synthesis, two examples: 1. Hydrolysis of Benzamide 2. Oxidation of Toluene

12 experiments will be notified by HOD from time to time

**Reference Books**

1. Vogel A.I. – “Text book of practical organic chemistry”, 5<sup>th</sup> Ed. ELBS, London, 1989.
2. Dey B.B. and Sitharaman M.V., “Laboratory manual of Organic Chemistry” Revised by T.R. Govindachari, Allied Publishers Ltd., New Delhi, 4<sup>th</sup> Revised edition, 1992.
3. Palleros Daniel R., “Experimental Organic Chemistry” John Wiley & Sons, Inc., New York, 2000.
4. Fumiss B.S., Hannaford A.J., Rogers V., Smith P.W.G. and Tatchell A.R., “Text book of Practical Organic Chemistry”, LBS, Singapore, 1994.
5. Khopar S.M., “Basic concepts of Analytical Chemistry”, John Wiley & Sons, 1984.

**12CH220 CHEMISTRY IN EVERYDAY LIFE**

**Credits 3:0:0**

**Course Objective:**

- To introduce to the students about the chemistry connections of everyday life.

- To relate what the student studies in the subjects to practical life.

### Course Outcome:

- The students will know the practical aspects of chemistry in day-to-day life.
- The students will think innovative and develop application oriented products.

### Unit 1

**DRUGS AND DISEASES:** Clinical chemistry – Antibiotics, antiseptics, antipyretics – Definitions, examples (common drugs available in the market) – Incurable diseases – Causes for polio, diabetes, AIDS, cancer – Signs and symptoms – Vaccination – Protein misfolding and disease – Common drugs banned in India – Effects of using banned drugs – Effects of steroidal injections.

### Unit 2

**PERFUMES, EXPLOSIVES, AND DYES:** Perfumes: historical significance – The olfactory system – Categories – Chemistry of ice cream making – Chemistry of paint – Chemistry of explosives – TNT, RDX, nitrocellulose, nitroglycerine (structure and properties only) – Natural dyes and synthetic dyes – Types, advantages, applications – Hair dye – Petrochemicals.

### Unit 3

**CHEMICALS IN EVERYDAY PRODUCTS:** Advantages and disadvantages of the following: monosodium glutamate (aginomotto) – Lycopene (in tomato) – Umami, the fifth taste and glutamate – Caffeine and theobromine (in chocolates) – Polyphenols (in tea) – docosahexanoic acid (in fish) – Thiols (in onion) – Polycyclic aromatic hydrocarbons (formed during cooking meat) – Constituents of talcum powder and pulmonary fibrosis – Ingredients of tooth paste – Melatonin (in anti-ageing product) – Microban (in toys) – Alpha tocopherol (in body lotions) – Aluminum chloride (in antiperspirants) – Aspartame (in artificial sweetener) – Chloral hydrate (in sedatives) – Citric acid (in citrus fruits).

### Unit 4

**CHEMICAL BASIS OF EVERYDAY PHENOMENA:** Chemical basis of everyday phenomena – Reasoning: kitchen gas burner burns yellow when a pot of boiling water overflows – Cosmetic creams feel cool when applied to skin – Seashells vary in color – Old paintings discolor over time – Hair color products remove gray on hair – Disappearing inks disappear – Water does not relieve the burning sensation of chilly – Sniffing dogs detect explosives and bombs – Flesh of fish smells different from other meat – Puff pastries expand when prepared – some fabrics are water-repellent – Cotton is highly water absorbent but dries slowly.

### Unit 5

**KNOWING CHEMISTRY FOR BETTER LIFE:** Food adulteration – Consumption of alcohol and its ill effects – PAH from oil – Balanced diet – Iodized salt – Fluoride tooth paste – Saturated and unsaturated fat - Cholesterol (LDL and HDL) – Ill health and fast food – Organic food – crackers – ill effects of crackers – Molecules of emotion (Adrenaline, Acetylcholine, Dopamine, Epinephrine, Norepinephrine, Serotonin, Melatonin, Oxytocin).

### Text Books

- 1 Karukstis K.K., and Hecke G.R.V., “Chemistry connections: the chemical basis of everyday phenomena” Elsevier Science and Technology books, 2nd edition, 2003.

- 2 Grace Ross Lewis, "1001 Chemicals in everyday products", John Wiley and sons, 3rd edition, 2001.

## References

- 1 [www.listverse.com/2007/10/04/top-10-incurable-diseases/](http://www.listverse.com/2007/10/04/top-10-incurable-diseases/)
- 2 [www.bama.ua.edu/](http://www.bama.ua.edu/)
- 3 [www.foodproductdesign.com](http://www.foodproductdesign.com)
- 4 [www.angelfire.com/linux/chemistryofpaint/](http://www.angelfire.com/linux/chemistryofpaint/)
- 5 [www.srsi.org/sr1/weapon.explode.htm](http://www.srsi.org/sr1/weapon.explode.htm)
- 6 Paul Engel, "Pain-free Biochemistry", Wiley – Blackwell publishers, 2009.

## 12CH301 ORGANIC CHEMISTRY – I

**Credits: 4:0:0**

### Course objective:

- To enable the student to understand (a) The stereochemistry of organic reactions (b) The detailed mechanism of all kind of organic reactions.

### Course Outcome:

- Students can carryout organic reactions with proper understanding and knowledge of mechanism and orientation changes.

### Unit I

**REACTION MECHANISM – I:** Effect of structure and reactivity – Resonance and field effects – Steric effects – Quantitative treatments of the effect of structure and reactivity – LFER – Hammett and Taft equation - Importance of  $\sigma$  and  $\rho$  values in aromatic electrophilic substitutions – Labelling and kinetic isotopic effects. Aromaticity – Huckel's rule – Aromatic systems with electron numbers other than six – Annulenes and Hetero annulenes.

### Unit II

**REACTION MECHANISM – II:** Aliphatic nucleophilic substitution – Mechanisms –  $S_N2$ ,  $S_N1$ , mixed  $S_N1$  and  $S_N2$ ,  $S_{Ni}$ ,  $S_{ET}$ , Neighbouring group mechanism – Reactivity – Effect of substrate, attacking nucleophile, leaving group and reaction medium – Substitution at vinylic and allylic carbons. Aromatic nucleophilic substitutions – Mechanism –  $S_{NAr}$  –  $S_{N1}$  – Benzyne – Reactivity – Effect of substrate, leaving group and attacking nucleophile.

### Unit III

**REACTION MECHANISM – III:** Aromatic electrophilic substitution – Arenium ion mechanism – Orientation and reactivity in monosubstituted benzene rings – Benzene rings with more than one substituent - Effect of leaving group – o/p ratio – Addition to C-C-multiple bonds – Mechanisms – Electrophilic, nucleophilic, free radical – Orientation and reactivity – Addition to conjugated systems – Elimination – Mechanisms of  $\beta$  elimination – ( $E_2$ ,  $E_1$ ,  $E_{1CB}$ ) –  $E_1$  –  $E_2$  –  $E_{1CB}$  spectrum, orientation of double bonds – Reactivity – Effect of substrate, attacking base, leaving group and medium.

### Unit IV

**STEREOCHEMISTRY – I:** Stereoisomerism – Definitions and classification – Molecular representation and inter conversion – Classification of stereo isomers – Stereoisomerism and

center of chirality – Molecules with a single stereogenic center – Projection structure of stereoisomers – Fischer – DL, RS and EZ notations - Configurational nomenclature – Molecules with two or more chiral centers – Stereoisomerism in cyclic compounds – Axial chirality, planar chirality and helicity.

### Unit V

**STEREOCHEMISTRY – II:** Difference between conformation and configuration – Conformation of ethane, substituted ethanes – Conformation of cyclohexanes, mono, and disubstituted cyclohexanes – Saw-horse, staggered, skew, gauche forms – Explanation and conversion of one representation to another – Fused ring systems – Decalins – Biphenyls - Stereoisomerism in Allenes Dynamic stereochemistry: Stereoselectivity and stereospecificity – Curtin-Hammett principle – Enantioselective, diastereoselective synthesis – Enzymatic and kinetic methods – Conformation and reactivity in acyclic compounds and cyclohexanes.

### Text Books

1. Jerry March, “Advanced Organic Chemistry”, Wiley Eastern Limited, New Delhi, 4th edition, 2008.
2. Bahl. B.S. and Arun Bahl, “A Text book of Organic Chemistry”, S. Chand & company Ltd., New Delhi, Reprint, 2011.
3. Peter Skyes, “A Guidebook to Mechanism in Organic Chemistry”, Longman Press, London and New York, Reprint, 2006.
4. Ernest. L. Eliel, “Stereochemistry of carbon compounds”, Tata-McGraw Hill, New Delhi, 22nd Reprint 2009.

### Reference Books

1. Nasipuri. D. “Stereochemistry of organic compounds – Principles and applications”, New Age international, 2nd edition, 2002.
2. Kalsi. P.S. “Stereochemistry Conformation and Mechanism”, New Age International Publishers, New Delhi, 6th Edition, Reprint, 2005.
3. Finar. I.L., “Organic Chemistry, Volume 1”, Doorling Kindersley (Indian), 6th Edition, 5th impression, 2008.
4. Raj K. Bansal, “Organic reaction mechanism”, Tata McGraw Hill, New Delhi, 4th Edition, 2005.
5. Cary. F.A. “Organic Chemistry”, McGraw Hill, Inc., 2nd edition, 1992.
6. Morrison and Boid, “Organic Chemistry”, United States of America, 3rd edition, 1992.

## 12CH302 PHYSICAL CHEMISTRY – I

**Credits: 4:0:0**

### Course Objective:

- To know about Classical & Statistical thermodynamics.
- To know about Phase rule for one component, two component and three component systems.
- To know about Surface chemistry.

### Course Outcome:

- Students acquire a good understanding of the basic principles of Classical and Statistical

thermodynamics, application of phase rule to different chemical systems and the importance of Surface chemistry.

### Unit I

**CHEMICAL THERMODYNAMICS:** First law of thermodynamics – Limitation of first law of thermodynamics - Second law of thermodynamics – Third law of thermodynamics – Entropy – Entropy change in phase transformations – Entropy changes of an ideal gas in different processes – Entropy at absolute zero – Determination of absolute entropies of solids, liquids and gases – Trouton's rule - Partial molar properties – Chemical potential – Gibbs – Duhem equation – Variation of chemical potential with temperature and pressure – Activity – Activity coefficient – Ideal solution – Real solution – Fugacity – Determination of a fugacity of a gas.

### Unit II

**PHOTOCHEMISTRY:** Absorption and emission of radiation – Theories – Spontaneous and induced emission – Laser – Franck Condon principle - Type 1 & 2 – Physical properties of electronic excited state – Emission – Resonance emission – Selection rule – Fluorescence – Phosphorescence – Delayed fluorescence: E-Type and P-Type – Excimer and Exciplex complex formation – Photosensitization and Chemiluminescence – Experimental techniques – Actinometry – Chemical actinometry – Flash photolysis.

### Unit III

**PHASE RULE:** Gibbs phase rule and phase equilibria – Degree of freedom – One component system – Water system – Sulphur system – Carbon-di-oxide system – Two components system – Reduced phase rule – Lead-silver system – Pattinson's process – Ferric chloride-water system – Potassium iodide-water system – Sodium chloride-water system – Copper-nickel alloy system – Tin-lead alloy system – Three component system – Brief description about two salts and water system – Allotropy.

### Unit IV

**STATISTICAL THERMODYNAMICS – I:** Concepts of probability and Maxwell Boltzmann distribution – Basic derivation – prove that  $\beta = 1/KT$  – Relationship between entropy and thermodynamic probability systems with degeneracy – Definitions of partition function – applications – derivation of thermodynamic functions from partition function – entropy for monoatomic gases – Sackur – Tetrode equation – The Bose – Einstein's system – Basic derivation – Fermi – Dirac system – Basic derivation.

### Unit V

**STATISTICAL THERMODYNAMICS – II:** Heat capacity of solids – Debye and Einstein models – Irreversible thermodynamics – the steady – coupled flows – application – over potential – decomposition potential – electrical double layer – structure of electrical double layer – capacity – steaming potential – electro dialysis – the Dorn effect

### Text Books

1. Atkins P.W., "Physical Chemistry", Oxford University Press, 8th edition, 2006.
2. Puri B.R., Sharma L.R. and Madan S. Pathania, "Principles of Physical Chemistry", Shoban Lal Nagin Chand & Co., Jalandhar, 2002.
3. Rohatgi Mukherjee K.K., "Fundamentals of photochemistry", New Age International Pvt. Ltd., New Delhi, 2009.
4. Glasstone S., "Thermodynamics for Chemists", East West Press Pvt. Ltd., New Delhi, 2005.

## Reference Books

1. Kapoor K.L., "A Text Book of Physical Chemistry" Vol. II Macmillan India Ltd., 3rd edition, 2005.
2. Levine I.N., "Physical Chemistry", Tata Mac Graw Hill, NY, 2007.
3. G.W. Castellan, "Physical Chemistry", Narosa Publishing House, Chennai, 2004.
4. N.D. Smith, "Elementary Statistical Thermodynamics", Plenum Press, New York, 1984.
5. Alan Cox and T.J. Kemp, "Introductory photochemistry", McGraw-Hill, 1971.

## 12CH303 INORGANIC CHEMISTRY – I

**Credits: 4:0:0**

### Course Objective:

- The various bonding theories in inorganic chemistry will be discussed.
- Background on inorganic chemistry as applied to solid state chemistry will be discussed.
- The student will study the detailed account of nuclear chemistry and their application in various fields.
- The student will understand the principles of metallurgy and will study the importance of lanthanides and actinides in detail.

### Course Outcome:

- The student will get the thorough knowledge of various bond theories, solid state chemistry, Nuclear chemistry, metal extraction techniques and the various properties of lanthanides and actinides.

### Unit I

**STRUCTURE AND BONDING:** Ionic bond – Formation – Characteristics of ionic compounds - Melting point, boiling point, hardness, electrical conductivity and solubility – Structure of crystal lattices – Lattice energy - Born-Landé equation and Born Heber Cycle – Polarization of ions - Fajan's rule – Calculation of some limiting ratio values – Covalent bond – Rules for covalent bond formation – Valence bond theory – Resonance and hybridization – Molecular orbital theory and its application in diatomic molecules – Comparison of VB and MO theories – Bond properties – Bond energy – Bond length – Bond polarity – Electron pair repulsion theory and its applications – Hydrogen bond – Types – Effect on molecular properties – Detection of hydrogen bonding.

### Unit II

**SOLIDS:** Bond theory of solids – Electrical properties – Insulators – Semiconductors – Superconductors – Dislocation in solids – Schottky and Frenkel defects – Structure of some compounds of AX, AX<sub>2</sub> and AMX<sub>2</sub> types – Perovskite, Ilmenite and Spinel structures.

### Unit III

**NUCLEAR CHEMISTRY:** Modes of radioactive decay and rate of radioactivity decay – Radioactive detectors – Types of nuclear reactions – Artificial radioactivity – Nuclear stability – Packing fraction – Mass defects and binding energy – Nuclear fission of uranium - Liquid drop model – Nuclear fusion – Essential features of water cooled thermal reactors and fast breeders – Neutron activation analysis – Carbon and rock dating – Applications of tracers in chemical analysis, reaction mechanisms, medicine and industry.

#### Unit IV

**METALLURGY:** Isolation, purification, properties and uses of Beryllium, Germanium, Titanium, Zirconium, Thorium, Vanadium, Uranium and Platinum. – Preparation and uses of the following compounds - Basic Beryllium acetate,  $\text{BeCl}_2$ ,  $\text{TiCl}_4$ ,  $\text{TiO}_2$ , Titanium isopropoxide,  $\text{ZrCl}_4$ , Zirconia,  $\text{V}_2\text{O}_5$ ,  $\text{VCl}_4$ ,  $\text{UF}_4$ , Uranyl nitrate,  $\text{ThO}_2$ ,  $\text{Th}(\text{NO}_3)_2$ ,  $\text{PtCl}_4$  and  $\text{H}_2\text{PtCl}_6$

#### Unit V

**CHEMISTRY OF LANTHANIDES AND ACTINIDES:** Lanthanides – Position in the periodic table – General properties of lanthanides and actinides – Electronic configuration, oxidation state and oxidation potential, atomic and ionic radii – Cause and consequences of lanthanide and actinide contractions – Comparison of spectral and magnetic properties of lanthanide and actinide complexes – Chemistry of their important compounds: Oxides, nitrates and sulphates.

#### Text Books

1. Cotton F. A & Wilkinson G, “Advanced Inorganic Chemistry”, 6th edition, Wiley India (P.) Ltd, New Delhi, India, First Reprint 2007.
2. Lee J. D, “Concise Inorganic Chemistry”, 5th edition, Wiley India (P.) Ltd, New Delhi, India, Reprint: 2009.
3. Satyaprakash, Tuli G. D, Basu S. K & Madan R. D, “Advanced Inorganic Chemistry” Vol I and II, S. Chand and Company Ltd, New Delhi, India, Reprint: 2009.

#### Reference Books

1. Shriver and Atkins, “Inorganic Chemistry”, Oxford University Press, New Delhi, India, 4th edition, 2009.
2. Greenwood N. N & Earnshaw A, “Chemistry of the Elements”, Reed Elsevier India Private Ltd, Gurgaon, India, 2nd edition, Reprinted 2010.
3. West R, “Solid State Chemistry and its Applications”, Wiley India Pvt. Ltd, New Delhi, India, 2007.
4. Arnikaar H. J, “Essentials of Nuclear Chemistry”, New Age International Publishers Ltd., New Delhi, India, 4th edition, 2007.
5. Sharpe A.G. “Inorganic Chemistry”, Dorling Kindersley (India) Pvt. Ltd, 2nd impression, 2008.

### 12CH304 ORGANIC CHEMISTRY – II

**Credits 4:0:0**

#### Course Objective:

- To enable the student to understand (a) The principles of organic synthesis (b) Reagents used in organic synthesis (c) Photochemical, Pericyclic, and different Molecular rearrangements.

#### Course Outcome:

- Students can make use of different reagents in organic synthesis and they can do it in different pathways.

## Unit I

### **ORGANIC NAME REACTIONS AND REAGENTS USED IN ORGANIC SYNTHESIS:**

Organic name reactions – Wittig Reaction – Michael addition - Mannich reaction - Stork Enamine reaction – MPV reduction, Oppenauer oxidation, Ene reaction - Barton reaction - Chichibabin reaction - Fischer – Indole synthesis – Complex metal hydrides – NaBH<sub>4</sub>, LiAlH<sub>4</sub>, NaCNBH<sub>3</sub>, Gilman's reagent - Lithium dimethylcuprate - Lithium diisopropylamide (LDA)- Osmium tetroxide – DDQ - Selenium dioxide - Merrifield resin.

## Unit – II

**MOLECULAR REARRANGEMENTS:** Mechanism of the following rearrangement reactions – Favorskii rearrangement - Pinacol-Pinacolone rearrangement – Wagner-Meerwein rearrangement– Hofmann rearrangement– Beckmann rearrangement – Curtius rearrangement – Wolff rearrangement – Baeyer-Villiger reaction – Dakin reaction – Stevens rearrangement – Sommelet rearrangement – Wittig rearrangement – Benzidine rearrangement– Benzil-Benzilic acid rearrangement – Cope rearrangement – Dienone rearrangement.

## Unit III

**ORGANIC PHOTOCHEMISTRY:** Distinctive feature of Photochemical reactions – Absorption of light by organic molecules – Excited states – Transfer of excitation energy – Bimolecular Processes - Sensitization and quenching – Photochemical eliminations, Norrish type I and II reactions, Paterno-Buchi reaction, cis-trans isomerisation, rearrangements (di-pi methane or Zimmerman rearrangement).

## Unit IV

**PERICYCLIC REACTION:** Definition – Types – Woodward-Hofmann rules, Orbital correlation diagrams, FMO treatment, PMO method, Electrocyclic conversion of 1,3-dienes and 1,3,5-trienes – Cycloadditions – 2+2 addition, Diels-Alder reaction, Sigmatropic reactions – Cope and Claisen rearrangement – Olefin Metathesis – Grubbs Catalyst.

## Unit V

**RETROSYNTHESIS – THE DISCONNECTION APPROACH:** Synthons and reagents – Strategy I : The order of events – one group disconnection – Strategy II : Chemoselectivity – Two group Disconnection – Strategy III: Reversal of polarity and cyclization – Strategy IV: protecting groups – Strategy V : Stereoselectivity – Strategy VI : Carbonyl condensation - Strategy VII : Aliphatic nitro compounds – Strategy VIII: Ring synthesis.

## Text Books

1. Stuart Warren, "Organic Synthesis – The disconnection approach" – A John Wiley and Sons, Ltd., 2nd Edition, reprint, 2010.
2. Jagadamba Singh and Jaya Singh, "Photochemistry and Pericyclic Reactions", New Age International Publishers, New Delhi, 3rd Revised Edition, Reprint, 2011.
3. Carey, F.A, and Sundberg. R. J, "Advanced Organic Chemistry Part – B: Reactions and Synthesis", Plenum Press, 2008.
4. Gurdeep R. Chatwal, "Reaction Mechanism and Reagents in Organic Chemistry", Himalaya Publishing House, New Delhi, 2007.

## Reference Books

1. Finar. I.L, "Organic Chemistry", Volume 2, Doorling Kindersley (Indian), 6th Edition, 5th impression, 2008.

2. Chatwal. G. R, "Organic Photochemistry", Himalaya Publishing House, Mumbai, 1st Edition 2008.
3. Hassner. A, and Stumber. C, "Organic Synthesis based on name reactions", Pergamon Press, 2002.
4. Ahluwalia. V. K, and Rakesh Kumar Parashar, "Organic Reaction Mechanisms", Narosa Publishing House, New Delhi, 4th Edition, 2011.
5. Gilchrist. T. L, & Storr. R.C, "Organic reaction orbital symmetry", Cambridge university press, 1979.
6. Jerry March, "Advanced Organic Chemistry – Reactions, Mechanisms and structure", John Wiley & Sons, 4th Edition, 2008.
7. Mukherji. S. M, and Singh. S.P, Reaction Mechanism in Organic Chemistry, Macmillan Publishers, 3rd Edition, Reprinted, 2010.
8. Coxon. J.M, and Halton. B, "Organic Photochemistry", Cambridge University Press, London, 1st Paper back edition, 2011.

## 12CH305 PHYSICAL CHEMISTRY – II

**Credits: 4:0:0**

### Course Objective:

- To know about chemical kinetics, mechanism of gas phase reactions, catalysis & quantum mechanics.

### Course Outcome:

- Students acquire a good knowledge on the chemical kinetics, mechanism of gas phase reactions, catalysis and quantum chemistry of atoms and molecules.

### Unit I

**CHEMICAL KINETICS - I:** Chemical kinetics – Basic concepts – rate law – rate equation – Kinetics of zero, first, second and third order reactions – Kinetics – composite reactions (complex reaction) – Opposing (reversible) reactions – Consecutive reactions – Chain reactions – Stationary chain reaction – Collision theory of bimolecular and unimolecular reactions – Arrhenius theory of reaction rates – Theory of absolute reaction rates – Thermodynamic treatment of reaction rate - Lindemann's theory – Kinetics of fast reactions.

### Unit II

**CHEMICAL KINETICS - II:** Study of kinetics of stopped flow techniques – flash photolysis – shock tubes – Reaction rates in solution – Effect of dielectric constant and ionic strength – Kinetic isotope effects – Hammett relationship - ionic reactions in solution – effect of ionic strength – Linear free energy relationships – Taft equation – Yukawa-Tsuno equation – Luminescence and energy transformations – Chemiluminescence – reactions in molecular beam.

### Unit III

**CATALYSIS:** Acid – Base catalysis – general scheme – Arrhenius complex – Vant Hoff's complex – specific and general catalysis – catalytic constants – Bronsted relationship – Hammett acidity functions – mechanism of acid-base catalysed reaction – Catalysis by metal salts (transition metal complex) – enzyme catalysis – theory and applications - Mechanism of heterogeneous catalysis - Langmuir-Hinshelwood mechanism and Langmuir Reidel mechanism -

Examples of heterogeneous catalytic reactions - hydrogenation of ethylene , synthesis of ammonia, oxidation of SO<sub>2</sub> and Fischer- Tropsch method for the synthesis of methanol.

#### Unit IV

**INTRODUCTION TO QUANTUM MECHANICS:** The failures of classical mechanism – heat capacities – black body radiation – The photo electric effect – The Compton effect – The diffraction of electrons – wave particles duality – Uncertainty principle, operators and commutation relations – Postulates of quantum mechanics – Scrodinger equation, Free particle, particle in one dimensional box, three dimensional box – Harmonic oscillator – Rigid rotor – The Schrodinger equation for hydrogen atom – Angular momentum – Spin, coupling of angular momentum – Spin-orbit coupling.

#### Unit V

**QUANTUM CHEMISTRY OF ATOMS AND MOLECULES:** Variation and perturbation theory – Application of perturbation / variation theorems to ground state of helium atom – Antisymmetry and Pauli's exclusion principle – Aufbau principle – Slater detrimental wave functions – Term symbols and spectroscopic states – Born Oppenheimer approximation – LCAO, MO and VB treatments of hydrogen molecule – Hybridization – Huckel theory of linear conjugated systems – Cyclic systems – Wood- ward Hoffman rules.

#### Text Books

1. Laidler K.J., "Chemical Kinetics", Harper and Row, New York, 3rd Edition, 2008.
2. Rajaram J., and Kuriakose, J.C., "Kinetics and mechanism of chemical transformation", McMillan India Ltd., New Delhi, 2011.
3. Adamson, A.W. , "Physical Chemistry of Surfaces", Wiley, 6th edition, 1997.
4. Chandra, A.K. "Quantum Chemistry" Tata McGraw – Hill Pvt. Ltd., New Delhi, 4th Edition, 2002.

#### Reference Books

1. Kalidas, C. "Chemical Kinetic Methods: Principles of Relaxations Techniques and application", New Age International (P) Ltd, Chennai, 2005.
2. Donald A McQuarrie, "Quantum Chemistry", Viva Books, New Delhi, 2008.
3. Hanna, M.W., "Quantum Mechanics in Chemistry", Addition Wisley, London, 3rd edition, 1981.

### 12CH306 INORGANIC CHEMISTRY – II

**Credits: 4:0:0**

#### Course Objective:

- Coordination Chemistry is the backbone of inorganic chemistry and the structure and reaction mechanisms of coordination complexes will be discussed.
- The various reaction mechanisms including substitution, electro-transfer and photochemical reactions will be discussed.
- The importance of main group chemistry will be discussed.

### Course Outcome:

- The student will get the thorough knowledge about the coordination chemistry. He will understand the various bonding theories in inorganic complexes and the types of mechanisms involved in coordination chemistry. He will also know the importance of main group chemistry.

### Unit I

**COORDINATION CHEMISTRY – STRUCTURE AND BONDING:** Introduction - Formation of complexes - Bonding theories for coordination complexes – Werner’s theory – Stability constant - Experimental determination of stability constant – Factors influencing – Stabilization of unusual oxidation states by complex formation – Crystal field theory – Concept, influence of ligand on CF splitting and limitation – Term symbols – Orgel diagram – Tanabe Sugano diagrams ( $d^1$  and  $d^4$ ) - Ligand field theory – Jahn – Teller effect – Electronic spectra and magnetic moments - Types of magnetic interactions -Recent techniques of magnetic susceptibility measurements - Low-spin – high-spin transitions - Molecular orbital theory of a complex and its limitation – Ligand Design – Chelate and macrocyclic Effect - Isomerism in Metal Complexes – Optical isomerism - Stereochemical nonrigidity.

### Unit II

**INORGANIC REACTION MECHANISMS – SUBSTITUTION REACTIONS:** Reactions of square planar complexes – Mechanism of ligand displacement reaction – Substitution in the square planar complexes - Mechanism, entering group effect, cis effect and trans effect - Thermodynamic and kinetic stability - Substitution in octahedral complexes – Dissociative and associative mechanisms – Base hydrolysis - Isomerisation reactions – Substitution without breaking the metal –ligand bond.

### Unit III

**INORGANIC REACTION MECHANISMS – ELECTRON TRANSFER REACTIONS:** Electron transfer reactions – Outer sphere and inner sphere mechanisms and rate laws - Various types of electron transfer reactions - Marcus-Husch theory - Correlation between thermal and optical electron transfer reactions - Identification of intervalence transfer bands in solution.

### Unit IV

**INORGANIC PHOTOCHEMISTRY:** Excited states of Coordination complexes - Properties of excited states - Photochemical pathways - Energy transfer, Charge transfer photochemistry, Photoredox reactions, Photosubstitution reactions - Ruthenium polypyridines - Ligand photoreactions - Photochemical conversion and storage of solar energy – Introduction to inorganic photochemistry at semiconductor electrodes.

### Unit V

**MAIN GROUP CHEMISTRY:** Preparation, structure and bonding of boron hydrides, carboranes and heteroboranes - Polymorphism of carbon, phosphorous and sulphur – Synthesis, structures and properties of silicates and carbides - Oxyacids of selenium and tellurium - Chalcogenide clusters - Homocyclic inorganic systems.

### Text Books

1. Huheey J. E, Keiter E. A & Keiter R. L, “Inorganic Chemistry – Principles of structure and reactivity”, Dorling Kindersley (India) Pvt. Ltd, New Delhi, India, 4th edition, 2009.

- Porterfield W. W, "Inorganic Chemistry A Unified Approach", Reed Elsevier India Private Ltd, Gurgaon, India, 2nd Edition, Reprinted 2009.
- Purcell K. F & Kotz J. C., "Inorganic Chemistry" Cengage Learning, New Delhi, India, Reprint, 2010.

### Reference Books

- Cotton F. A & Wilkinson G, "Advanced Inorganic Chemistry", Wiley India (P.) Ltd, New Delhi, India, 6th edition, First Reprint 2007.
- Miessler G. L & Tarr D. A., "Inorganic Chemistry", Dorling Kindersley (India) Pvt. Ltd, New Delhi, India, 3rd Edition, 2009.
- Douglas B. E, McDaniel D. H & Alexander J. J, "Concepts and Models of Inorganic Chemistry", Wiley India (P.) Ltd, New Delhi, India, 3rd edition, Reprint 2007.
- Jordan R. B, "Reaction Mechanisms of Inorganic and Organometallic Systems", Oxford University Press, New York, USA, 3<sup>rd</sup> Edition, 2007.
- Driess M. & Nöth H, "Molecular Clusters of the Main Group Elements", Wiley-VCH Verlag GmbH & Co, Weinheim, Germany, 2004.
- Figgis B. N. & Hitchman M. A, "Ligand Field Theory and Its Applications", Wiley-VCH Verlag GmbH & Co, Weinheim, Germany, 2000.
- Greenwood N. N. & Earnshaw A, "Chemistry of the Elements", Reed Elsevier India Private Ltd, Gurgaon, India, 2nd edition, Reprinted 2010.

## 12CH307 ORGANIC CHEMISTRY – III

Credits 4:0:0

### Course Objective:

- To enable the student to understand (a) Heterocyclic and supramolecular reactions (b) Natural products and its medicinal applications.

### Course Outcome:

- Students will be aware of natural products and its medicinal use; they will get an outlook about chemical modification of natural products for its further applications.

### Unit I

**HETEROCYCLES:** Nomenclature – Compounds containing two hetero atoms – Azoles – Chemistry of Pyrazole, Imidazole, Oxazole, Isoxazole, Thiazole and Isothiazole – Diazines – Chemistry of Pyridazine, Pyrimidines and Pyrazines.

### Unit II

**NATURAL PRODUCTS – I:** General methods of structure elucidation of alkaloids – Structure, synthesis and stereochemistry of the following alkaloids – Quinine, Morphine, Cocaine and Reserpine - Terpenoids - Classification - Structure, Stereochemistry and synthesis of Camphor, Zingiberene and Abietic acid.

### Unit III

**NATURAL PRODUCTS – II:** Vitamins – Introduction to vitamins A, B, C, D and E - Synthesis of Retinol and L-Ascorbic Acid. Introduction – Structure of anthocyanidins – General methods of synthesizing anthocyanidins - Cyanidin Chloride – Flavones – Flavonols - Iso flavones – Tannins.

#### **Unit IV**

**NATURAL PRODUCTS – III:** Steroids – Introduction, Nomenclature - Constitutional study of cholesterol, stereochemistry of steroids - Steroid hormones – Structural elucidation of Progesterone, Androsterone.

#### **Unit V**

**SUPRAMOLECULAR CHEMISTRY AND GREEN CHEMISTRY:** Introduction to Supramolecular chemistry – Molecular Recognition – Host-guest Chemistry – Self Assembly – Synthesis of Crown ethers and Calixarenes – Application of Cyclodextrins in Pharmacy – Green Chemistry - Principles – Ionic Liquids – Microwave Assisted Synthesis - Solid Support – Illustration with an example.

#### **Text Books**

1. Agarwal. O.P, “Chemistry of natural products, Vol.1 & 2”, Goel publishing house, 36th Edition, 2009.
2. Jonathan W. Steed, David R. Turner, Karl J. Wallace, “Core Concepts in Supramolecular chemistry and NanoChemistry” John Wiley & Sons Ltd, England, Reprint, 2007.
3. Raj.K. Bansal, “Heterocyclic Chemistry”, New Age International Publishers, 4th Edition, Reprint, 2009.
4. Rashmi Sanghi and M. M. Srivastava, “Green Chemistry Environmental Friendly Alternatives”, Narosa Publishing House, New Delhi, 4th Reprint, 2009.

#### **Reference Books**

1. Finar. I.L., “Organic Chemistry”, Volume 2, Doorling Kindersley (Indian), 6th Edition, 5th Impression 2008.
2. Jean-Marie Lehn, “Supramolecular Chemistry: Concepts and Perspectives” Paper Back Edition, 1995.
3. Gurdeep R. Chatwal, “Organic Chemistry of Natural Products”, Himalaya Publishing Home, New Delhi, 5th & Enlarged Edition, 2008.
4. Koichi Mikami, “Green Reaction Media in Organic Synthesis”, Blackwell Publishing Limited, UK, 1st published, 2005.

### **12CH308 PHYSICAL CHEMISTRY – III**

**Credits: 4:0:0**

#### **Course Objective:**

- To know about basics and applications of group theory.
- To understand the fundamental and applied concepts of photo chemistry, electrochemistry and nanotechnology.

#### **Course Outcome:**

- Students acquire knowledge on the basics of group theory, applications of group theory, practical applications of photochemical reactions, electrochemistry principles and nanotechnology.

### Unit I

**GROUP THEORY:** Molecular symmetry – symmetry elements and symmetry operations-successive operations, inverse operations - Cartesian coordinate system - relations among symmetry elements - Properties of a group – Abelian, non abelian and Isomorphic groups - Multiplication tables – classes, subgroups - Molecular point groups - Schoenflies symbols - Matrices of symmetry operations - Representations of a group-Reducible and irreducible, representations - Statement and proof of Great orthogonality theorem - Characters and construction of character table ( $C_{2v}$ ,  $C_{3v}$ ) – Explanation of a character table - Direct product groups.

### Unit II

**APPLICATIONS OF GROUP THEORY:** Standard reduction formula relating reducible and irreducible representations -Symmetries of normal modes of vibration in non-linear molecules ( $H_2O$ ,  $NH_3$ ,  $BF_3$ ) - Selection rules for vibrational spectra – IR and Raman active fundamentals – Mutual exclusion rule - Symmetries of M.O and symmetry selection rule for electronic transition in ethylene and formaldehyde - Hybridization schemes for atoms in methane, ethylene and butadiene.

### Unit III

**SURFACE CHEMISTRY:** Adsorption of gases by solids – Langmuir, Freundlich and B-E-T isotherms – Applicability to heterogeneous catalysis – Determination of surface area of adsorbents – Gibbs adsorption equation – Electrokinetic phenomena – Donnan membrane equilibrium – Emulsions.

### Unit IV

**INTRODUCTION TO APPLIED ELECTRO-CHEMISTRY:** Theories of electrical double layer (EDL) – EDL at the electrode – electrolyte interface- Helmholtz model of DL - Electrode kinetics – Butler Volmer equation–one step one electron transfer kinetics -Tafel equation and plots - Hydrogen overpotential – Mechanism of hydrogen evolution reactions – Theories of hydrogen overvoltage - Passivity (chemical and mechanical passivity) - Corrosion (definition, theory, methods of preventing corrosion) – Voltammetry – Experimental Techniques – Importance of Amperometric Titration – Introduction to Electrochemical energy conversions.

### Unit V

**NANO TECHNOLOGY:** Nanomaterials – Preparation: Plasma arcing - Chemical vapor deposition – Sol-gels – silica gels – Hydrolysis – Condensation and polymerization of monomers to form particles – Zirconia and yttrium gels – Aluminosilicate gels – Forming nanostructured surfaces using the sol – gel process – Trapping by sol –gels – Electrodeposition – Ball milling – Using natural nanoparticles – Applications of nano materials – Insulations materials - Machine tools – Phosphors – Batteries – High power magnets – Motor vehicles and aircraft – Medical applications.

### Text Books

1. Swarnalakshmi S. “A Simple Approach to Group Theory in Chemistry” Universities Press, 2009.

2. Raman, K.V. "Group theory and its applications to chemistry", Tata Mac Graw Hill, 2004.
3. Gabor A. Somorjai, "Surface Chemistry and Catalysis", John Wiley, NJ, 2010.
4. Samuel Glasstone, "An Introduction to Electrochemistry", Maurice Press, 2007.
5. Michael Wilson, Kamali Kannangara, Geoff Smith, Michelle Simmons and Burkhard Raguse, "Nanotechnology – Basic Science and Emergin Technologies", Chapman & Hall (CRC), 2004.

### Reference Books

1. Cotton F.A. "Chemical application of group theory", Wiley India Pvt. Ltd., New Delhi, India, 3rd edition, 2009.
2. Carter R.L., Molecular Symmetry and Group Theory, John Wiley & Sons, NY, 2005.
3. John O'M. Bockris, Amulya K. N. Reddy, "Modern Electrochemistry", Vol. I and II, Plenum Publishing, 2008.
4. Richard C. Alkire, Dieter M. Kolb, Jacek Lipkowski and Phil Ross, "Advances in Electrochemical Science and Engineering", Volume 9, Wiley, 2006.
5. Desai, K.R., Surface Chemistry, Oxford Book Company, Jaipur, 2008.

## 12CH309 INORGANIC CHEMISTRY – III

**Credits: 4:0:0**

### Course Objective:

- The frontier areas in inorganic chemistry will be discussed.
- The application of organometallic complexes in various fields and the role of metals in biology will be discussed.
- The student will study the detailed account of inorganic polymers.
- The role of metals in nanotechnology and the importance of various nanoparticles and their application will be discussed.

### Course Outcome:

- The student will get the thorough knowledge about the nonaqueous solvents, the synthesis and application of organometallic complexes and the importance of bioinorganic chemistry, the use of inorganic polymers and the importance of inorganic chemistry in nanotechnology.

### Unit I

**NONAQUEOUS SOLVENTS:** General properties and classification of solvents – Self-ionization and leveling effect – Reactions in nonaqueous solvents – Solute-solvent interaction - Reactions in liquid NH<sub>3</sub> – Solutions of metals in liquid ammonia – Reactions in acetic acid, anhydrous sulphuric acid, liquid SO<sub>2</sub>, liquid HF, interhalogens and liquid dinitrogen tetroxide – Titrations in nonaqueous solvents – Acid-base titrations.

### Unit II

**ORGANOMETALLICS:** Definition – Types of bonds – Metal carbonyls – Metal Nitrosyls - Complexes of olefin, acetylene, cyclopentadiene and benzene derivatives – Metallocenes – Fluxional molecules – Reactions – Coordinative unsaturation - Substitution, Oxidative addition, Reductive elimination, Insertion - Reactions of coordinated ligand – Catalysis - Hydrogenation, Carbonylation, Hydroformylation, Wacker Process and Ziegler-Natta Catalysis

### Unit III

**BIO-INORGANIC CHEMISTRY:** Essential and trace metals in biological systems – Metalloporphyrins – Chlorophyll, hemoglobin, myoglobin and vitamin B<sub>12</sub> – Iron sulphur proteins – Hydrogenase - Nitrogen cycle, nitrogen fixation and dinitrogen complexes – Metal centered enzymes – structure and function – Role of metal complexes in medicine - Anticancer drugs - Platinum complexes and their mechanism of action.

### Unit IV

**INORGANIC POLYMERS:** Classification, Types of Inorganic Polymerization - Comparison with organic polymers – Structure, properties and uses of inorganic polymers - Boron-oxygen and boron-nitrogen polymers – Polyphosphazenes - Silicones - Sulfur-nitrogen and sulfur-nitrogen-fluorine compounds – Coordination polymers.

### Unit V

**NANOMATERIALS:** General introduction - Synthesis of nanoparticles of gold and silver - Synthesis of nanoparticle semiconductors (TiO<sub>2</sub> and Fe<sub>2</sub>O<sub>3</sub>) - Nanowires and nanorods - Self-assembled nanostructures - Self-assembly and bottom-up fabrication – Graphenes, fullerenes and nanotubes - Applications of nanoparticles.

### Text Books

1. Cotton F.A & Wilkinson G, “Advanced Inorganic Chemistry”, Wiley India (P.) Ltd, New Delhi, India, 6th edition, First Reprint 2007.
2. Puri B. R, Sharma L. R & Kalia K. C, “Principles of Inorganic Chemistry”, Milestone Publishers and Distributors, New Delhi, India, 31<sup>st</sup> Edition, 2008.
3. Purcell K. F & Kotz J. C, “Inorganic Chemistry” Cengage Learning, New Delhi, India, Reprint 2010.

### Reference Books

1. Huheey J. E, Keiter E. A & Keiter R. L, “Inorganic Chemistry – Principles of structure and reactivity” Dorling Kindersley (India) Pvt. Ltd, New Delhi, India, 4th edition, 2009.
2. Shriver & Atkins, “Inorganic Chemistry”, Oxford University Press, New Delhi, India, 4<sup>th</sup> edition, 2009.
3. Gupta B. D & Elias A. J, “Basic Organometallic Chemistry”, CRC Press, New Delhi, India, 2010.
4. Bertini I, Gray H. B, Lippard S. J & Valentine J. S, “Bioinorganic Chemistry”, Viva Books Private Ltd, New Delhi, India, 2007.
5. Archer R. D, “Inorganic and Organometallic Polymers”, John Wiley and Sons, New York, USA, 2001.
6. Zhong Cao G, “Nanostructures and Nanomaterials: Synthesis, Properties and Applications”, Imperial College Press, London, United Kingdom, 2004.
7. Mido Y, Taguchi S, Sethi M. S & Iqbal S. A, “Chemistry in Aqueous and Non-Aqueous solvents” Discovery Publishing House, New Delhi, India, 2003.

## 12CH310 INORGANIC CHEMISTRY LAB

Credits: 0:0:4

### Course Objective:

- To provide the students an appreciation for the synthesis of Inorganic Complexes.
- To provide the students a competence in the laboratory skills required for accurate and precise chemical analysis.
- The students will know the theoretical basis of qualitative inorganic analysis containing common and less common ions.

### Course Outcome:

- The student will gain the laboratory skills to synthesize the inorganic complexes, to estimate the amount of metals quantitatively by complexometric and redox titrations and will be confident in analyzing the mixtures containing common and less common ions using semimicro analysis.

### INORGANIC COMPLEX PREPARATIONS (Any six)

- Hexathiourea Lead (II) nitrate
- Trithiourea Copper(II) chloride dehydrate
- Pentakis(thiourea) dicopper(I) nitrate dehydrate
- Potassiumtrioxalato ferrate (III)
- Bisglycinatecopper(II) monohydrate
- Hexamminecobalt(III) chloride
- Chloropentaamminecobalt (III) chloride
- Nitritopentamminecobalt (III) chloride
- Nitropentamminecobalt (III) chloride

### TITRATIONS (Any six)

- Estimation of Zinc by EDTA titrations
- Estimation of Calcium by EDTA titrations
- Estimation of Nickel by EDTA titrations
- Estimation of  $\text{Fe}^{2+}$  using redox titrations
- Estimation of Aluminium by EDTA titration (Back titration)
- Estimation of Nickel by EDTA titration (Back titration)
- Estimation of Lead by EDTA titration
- Estimation of Chromium by redox titrations

### INORGANIC QUALITATIVE ANALYSIS (Any eight)

Inorganic qualitative analysis experiments containing two common and two less common ions.

### Text Books

1. Mendham J., Denny R. C., Barnes J. D. and Thomas M. J. K., "Vogel's Textbook of Quantitative Chemical Analysis", 6th edition, Dorling Kindersley (India) Pvt. Ltd, New Delhi, India, Seventh impression 2008.
2. Ramanujam V. V., "Inorganic semimicro qualitative analysis", 3rd edition, The national publishing company, Chennai, India, reprinted 2008.

**Reference Book**

1. Svehla G., "Vogel's Textbook of Qualitative Chemical Analysis", 6th edition, Dorling Kindersley (India) Pvt. Ltd, New Delhi, India, fifth impression 2008.

**12CH311 ORGANIC CHEMISTRY LAB****Credits: 0:0:4****Course Objective:**

- To enrich the knowledge of Organic Laboratory skills for single step preparation, estimation and analysis of Organic mixture.

**Course Outcome:**

- Students acquire the knowledge of synthesis, estimation and analysis of Organic Compounds.

**EXPERIMENT A: SINGLE STEP PREPARATION**

- Preparation of Acetanilide From aniline (Acetylation)
- Preparation of Salicylic acid from Methyl-salicylate (Hydrolysis)
- Preparation of bromoacetanilide from acetanilide (Bromination)
- Preparation of p-nitroacetanilide from acetanilide (Nitration)
- Preparation of Picric acid from Phenol (Nitration)
- Preparation of benzanilide from aniline (Benzoylation)

**EXPERIMENT B: ESTIMATION**

- Estimation of aniline
- Estimation of Phenol
- Estimation of Dimethylketone
- Estimation of Ascorbic acid
- Estimation of Glucose (Bertrand's method)
- Estimation of Saponification value of oil

**EXPERIMENT C: SEPARATION OF BINARY MIXTURE AND ANALYSIS**

- Six experiments will be conducted with six different binary mixtures

**Text Book**

1. Gnanapragasam N.S., Ramamurthy G, "Organic Chemistry Lab Manual", revised edition, S. Viswanathan printers and publishers Pvt. Ltd., Chennai, Reprinted 2011.

**12CH312 PHYSICAL CHEMISTRY LAB****Credits: 0:0:4****Course Objective:**

- To carryout simple chemical reaction which would be monitored by Electrical and Non-Electrical experimental studies.

**Course Outcome:**

- The analytical skill will be improved by pursuing electrical experiments like Conductometry, Spectrophotometry, Potentiometry.
- The basic knowledge could be understood thoroughly regarding the velocity of the reaction, distribution properties and adsorption studies.

**ELECTRICAL EXPERIMENTS**

- Determination of Standard Electrode Potential
- Determination of solubility and solubility product of sparingly soluble salt

**ACID-BASE TITRATION – CONDUCTOMETRY**

- Strong base Vs Strong acid
- Strong base Vs mixture of Strong and Weak acids

**REDOX TITRATIONS -- POTENTIOMETRY**

- Potassium Dichromate Vs Ferrous Ammonium Sulphate
- Potassium Permanganate Vs Ferrous Ammonium Sulphate

**PRECIPITATION TITRATION -- POTENTIOMETRY**

- Silver Nitrate Vs Potassium Chloride
- Silver Nitrate Vs mixture of Halides

**NON-ELECTRICAL EXPERIMENTS**

- Determination of distribution coefficient and equilibrium constant of  $KI + I_2 \longrightarrow KI_3$
- Phase diagram – Simple Eutectic System
- Phase diagram – Compound formation

**KINETICS EXPERIMENTS**

- Ester Hydrolysis – Comparison of acid strength
- Ester Hydrolysis – Verification of Arrhenius equation

**ADSORPTION ISOTHERM**

- Freundlich Adsorption Isotherm – Verification

**SPECTROPHOTOMETRY**

- Estimation of Chromium – Verification of Beer's Law

**Text Book**

1. Svehla G., "Vogel's Textbook of Qualitative Chemical Analysis", 6th edition, Dorling Kindersley (India) Pvt. Ltd, New Delhi, India, fifth impression 2008.

**12CH313 ANALYTICAL CHEMISTRY – I****Credits: 4:0:0****Course Objective:**

- The student will learn how to analyze data and calculate error and the methods of separation of chemical compounds will be understood by him.
- Analysis of samples with IR, Electronic and Fluorescence spectroscopy and X-ray methods will be taught to the students.

### **Course Outcome:**

- The student will get theoretical background of chromatography techniques and will be able to analyze IR, electronic, fluorescence spectra and can determine the structures using X-ray Crystallography.

### **Unit I**

#### **INTRODUCTION TO ANALYTICAL METHODS AND CHROMATOGRAPHY**

**TECHNIQUES:** Errors - Accuracy and precision – Systematic and random errors – Significant figures and computation rules – Standard deviation - Correlation coefficient – Q test – Confidence interval - Chromatography: Principles and applications of Liquid column chromatography - Solid/liquid chromatography – Liquid/liquid chromatography - Ion exchange chromatography – Gel permeation chromatography - High Performance Liquid Chromatography - Gas chromatography.

### **Unit II**

**VIBRATIONAL SPECTROSCOPY:** General introduction to electromagnetic spectrum – IR spectroscopy – The vibrating diatomic molecule – Selection rule - The simple harmonic oscillator - Anharmonic oscillator - Vibrations of polyatomic molecules – Fundamental vibrations and overtones - Instrumentation – Sampling techniques - Factors influencing vibrational frequencies - Application to organic and inorganic compounds - Finger print region - Identification of functional groups - Simple problems in functional group identification using IR spectrum.

### **Unit III**

**ULTRAVIOLET AND VISIBLE SPECTROSCOPY:** Electronic spectroscopy of molecules - Electronic spectra of diatomic molecules - Physical principles – Chromophores and auxochromes - Laws of absorption – Absorption transitions - Instrumentation - Solvent effects - Applications of uv spectroscopy - Effects of conjugation - Woodward-Fieser rules -  $\alpha,\beta$ -Unsaturated carbonyl compounds, dienes, trienes and polyenes - Aromatic systems with extended conjugation – Heteroaromatic compounds - Simple problems – Absorption spectra of charge transfer complexes.

### **Unit IV**

**ORD, CD AND FLUORESCENCE SPECTROSCOPY:** Principles of optical rotatory dispersion (ORD) and circular dichroism (CD) – Cotton effect – Octant rule – Axial haloketone rule – Instrumentation - Applications of ORD and CD in organic and bio-molecules – Fluorescence Spectroscopy - Principles of Fluorescence – Jablonski diagram – Quantum yield – Collisional quenching – Stern-Volmer equation – Fluorescence Anisotropy – Steady state and time resolved fluorescence – Fluorescence polarization - Fluorescence resonance energy transfer — Fluorescence confocal microscopy.

### **Unit V**

**DIFFRACTION METHODS AND CRYSTALLOGRAPHY:** Laws of crystallography, Lattice types - X-ray diffraction - Bragg's equation – Instrumentation – Xray Diffraction Methods – Laue photographic method, Bragg method, Rotating crystal method, Powder method – Interpretation of diffraction pattern – Structure factor – Reliability factor - Applications of X-Ray Diffraction methods.

### Text Books

1. Chatwal G. R & Anand S. K, "Instrumental Methods of Chemical Analysis", Himalaya Publishing House, Mumbai, India, 5th Edition, Reprint 2011.
2. Banwell C. N. & McCash E. M., "Fundamentals of Molecular Spectroscopy", Tata McGraw-Hill Publishing Company Limited, New Delhi, 4th Edition, 2004.
3. Kemp W, "Organic Spectroscopy", PALGRAVE New York, 3rd Edition, 2008.
4. Williams D. H & Flemming I, "Spectroscopic Methods in Organic Chemistry", Tata McGraw-Hill Publishing Company Ltd, New Delhi, 5th Edition, 2004.

### Reference Books

1. Satya Narayana D. N, "Vibrational Spectroscopy Theory and Applications", New Age International Publishers, New Delhi, 2004.
2. Satya Narayana D. N, "Electronic Absorption Spectroscopy and Related Techniques", Universities Press (India) Ltd, Hyderabad, 2001.
3. Lakowicz J. R, "Principles of fluorescence spectroscopy", Springer Science+Business Media, New York, USA, 3<sup>rd</sup> editon, 2006.
4. Kalsi P. S, "Spectroscopy of Organic Compounds", New Age International Publishers, New Delhi, 6th Edition, 2004.
5. Willard H, Merrit L, Dean J. A. & Settle F.A., "Instrumental methods of chemical analysis", CBS Publishers and Distributers Pvt. Ltd, New Delhi, 7th edition, 1986.
6. Srivatsava A. K. & Jain P. C, "Chemical Analysis", S. Chand Publications, New Delhi, 3rd edition, 1997.
7. Skoog D. A, West D. M, Holler F. J & Crouch S. R, "Fundamentals of Analytical Chemistry", Cengage Learning India Pvt. Ltd, New Delhi, India, 8<sup>th</sup> Edition, 2004.

## 12CH314 ANALYTICAL CHEMISTRY – II

**Credits: 4:0:0**

### Course Objective:

- The student will understand the structure determination of organic molecules using NMR and Mass spectrometry.
- The Physical principles and applications of various analytical methods used by an inorganic chemist will be taught.
- Use of thermal methods and morphological studies for material chemists will be taught.

### Course Outcome:

- At the end of the semester the student will be confident to analyze the organic or inorganic complex molecules and also to characterize materials.

## Unit I

**NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY:** Theory- Nuclear spin-Interaction between spin and magnetic field - Population of energy levels - Larmor precession frequency - Relaxation processes – Instrumentation – Continuous wave and FT NMR - Proton nmr - Chemical shifts and its measurement – Reference compound – Factors affecting Chemical Shifts – Solvents used in NMR – Spin-spin coupling – Theory - Magnitude and factors affecting coupling constant - Long Range coupling – Second order spectra – AX, AMX, AB, AB<sub>2</sub> and ABX systems- Simplification of complex spectra - Applications of <sup>1</sup>H NMR to determine the structure of simple organic compounds - Introduction to Two Dimensional NMR (<sup>1</sup>H-<sup>1</sup>H COSY) spectroscopy.

## Unit II

**MULTINUCLEAR NMR SPECTROSCOPY AND ESR SPECTROSCOPY:** <sup>13</sup>C NMR spectroscopy- General Remarks – Operating frequency – Multiplicity – Broadband Decoupling – Off resonance decoupling – Line intensity – Chemical shifts – DEPT spectra – Applications of <sup>13</sup>C NMR to determine the structure of simple organic compounds - Introduction to <sup>19</sup>F, <sup>31</sup>P and <sup>29</sup>Si spectroscopy – ESR spectroscopy – Principle – g factor – Factors affecting intensity, position and multiplicity of spectra - Nuclear hyperfine structure – ESR spectra of simple organic radicals - Survey on spectra of first transition metal series (d<sup>1</sup>, d<sup>3</sup>, d<sup>5</sup>, d<sup>7</sup> and d<sup>9</sup> ions) – Zero field splitting – Kramer's degeneracy.

## Unit III

**MASS SPECTROMETRY:** Basic principles – Instrumentation – Molecular ion peak – Base peak – Isotopic abundance – Metastable ions – Nitrogen rule – General fragmentation modes – Factors affecting fragmentation – Mclafferty rearrangement – Retro-Diel's Alder reaction – Fragmentation and mass spectrum of organic compounds (Hydrocarbons, Halides, Alcohols and carbonyl compounds) – Introduction to GC-MS.

## Unit IV

**MOSSBAUER AND PHOTOELECTRON SPECTROSCOPY:** Mossbauer spectroscopy – Principles – Spectrometer – Chemical shift – Quadrupole effects – Effect of Magnetic field – Photoelectron spectroscopy – Photoionization process – Ionization energies – Spectra of diatomic molecules – Spectra of core electrons.

## Unit V

**THERMAL METHODS AND MORPHOLOGICAL STUDIES:** Introduction to thermal methods - Thermogravimetry (TG) – Differential Thermal Analysis (DTA) – Differential Scanning Calorimetry (DSC) – Theory – Instrumentation – Factors affecting TG, DTA and DSC Curves – Applications – Introduction to Surface characterization methods – SEM, FE-SEM, TEM – Sample characterization.

## Text Books

1. Kalsi P. S, "Spectroscopy of Organic Compounds", New Age International Publishers, New Delhi, 6th Edition, 2004.
2. Chatwal, Gurdeep R & Anand S. K, "Instrumental Methods of Chemical Analysis", 5<sup>th</sup> Edition, 2002, Himalaya Publishing House Mumbai, 2011.
3. Silverstein R. M. Webster F. X., "Spectroscopy of Organic Compounds", 6th Edition, Wiley Publications, 2009.

4. Satya Narayana D.N., "Magnetic Resonance Spectroscopy ESR, NMR, NQR", I. K. International, New Delhi, 2009.

### Reference Books

1. Banwell C. N & McCash, E. M, "Fundamentals of Molecular Spectroscopy", McGraw-Hill, New Delhi, 4th Edition, 2004.
2. William Kemp, "Organic Spectroscopy", PALGRAVE New York, 3rd Edition, 2008.
3. Williams D. H & Flemming I, "Spectroscopic Methods in Organic Chemistry", Tata McGraw-Hill Publishing Company Ltd, New Delhi, 5th Edition, 2004.
4. Willard, H, Merrit, L, Dean J.A & Settle F. A., "Instrumental Methods of Chemical Analysis", CBS Publishers and Distributors Pvt. Ltd, New Delhi, 7th edition, 1986.
5. Satya Narayana D. N, "Electronic Absorption Spectroscopy and Related Techniques", Universities Press (India) Ltd, Hyderabad, 2001.
6. Zhou W, Wang Z. L, "Scanning Microscopy for Nanotechnology: Techniques and Applications", Springer, New York, USA, 2006.

## 12CH315 POLYMER CHEMISTRY

**Credits 4:0:0**

### Course objective:

- To acquire the basic knowledge about the polymers.
- To understand the applications of polymers.

### Course Outcome:

- To understand the basic concepts of polymers.
- To know their properties and various fabrication techniques.
- To understand the new advanced materials like polymer nanocomposites and their applications.

### Unit I

**BASIC CONCEPTS OF POLYMERS:** Basic concepts of polymers – Classification of polymers – Tacticity – Structure property relationships – Naturally occurring polymers – Biopolymers – Introduction and types – Polysaccharides – Cellulose and proteins – Polymerization reactions – Classifications – Polymer resins – Polymer solutions – Reaction of polymers – Introduction of new groups – Cross linking, isomerisation, cyclisation and degradation reactions.

### Unit II

**PRINCIPLES OF POLYMERIZATION:** Principles and mechanisms of polymerization – Addition, step growth polymerization and coordination (i.e., Ziegler-Natta) – Reactivity of functional groups – Carothers equation – Kinetics – Characteristics of step growth polymerization – Examples – Mechanisms, choice of monomers, effect of inhibitors or retarders, – Co-polymerization – Monomer reactivity – Ratio – Composition, types, the Q-e scheme.

### Unit III

**POLYMER PROPERTIES:** Molecular weight determination methods – Polymer stereochemistry – Amorphous, crystalline and crystallites – Viscous flow – Viscosity – Thermal behavior of polymers –  $T_g$ ,  $T_m$  and their relationships – Elastic effect of polymers.

#### Unit IV

**POLYMERIZATION PROCESSES AND FABRICATION OF PLASTICS:** Polymerization processes – Bulk, solution, emulsion and suspension – Industrially important polymers and their polymerization processes – Polythene – Poly styrene – Nylon 6,6 – PET – PTFE – Natural rubber – Compounding of plastics – Additives added and their significance – Moulding processes – Injection, compression, blow moulding, extrusion moulding, thermoforming.

#### Unit V

**POLYMER NANO-COMPOSITES:** Introduction to – conducting polymers and composites, Applications in sensors, batteries – Conventional composites – Filler-matrix interaction, continuous (or long) and short fibre reinforced composites, laminates – Introduction to polymer nano-composites – Clay, CNT, particle filled – Advantages and limitations of nano fillers – Surface treatment on nano-fillers – Applications of polymer nano-composites – Packaging, automotive, mechanical components.

#### Text books

1. Gowariker, V.R., Viswanathan, N V and Jayadev Sreedhar, “Polymer Science”, I edition, New Age International Publishers Pvt. Ltd., New Delhi, India, Reprint 2008.
2. Misra, G.S., “Introductory polymer chemistry”, New Age International Pvt. Ltd., New Delhi, India, 1996, Reprint 2008.
3. Bahadur, P and Sastry, N V “Principles of polymer science” Narosa Publishing House Ltd., New Delhi, India, 2009.
4. Billmeyer, Jr, F W, “Textbook of Polymer Science” III edition, Wiley India Pvt. Ltd., New Delhi, India, 2007.

#### Reference books

1. Brydson, J.A. “Plastic materials” 4th edition, Butterworth –Heinmann Ltd., London, 1995.
2. Young, R J and Lovell, P A, “Introduction to Polymers” II Edition Reprint, Stanley Thornes (Publishers) Ltd., London 2000.
3. Seymour, R B, “Introduction to Polymer Chemistry”, Tata Mc GrawHill, New York, 1971.
4. Odian, G, “Principles of Polymerisation” IV Edition, Wiley Student Edition, New Delhi, 2007.
5. Arora, M Singh and Yadav, M S “Polymer Chemistry”, II revised Edition, Anmol Publications Pvt. Ltd., 2003.
6. Alexandre, M and Dubois, P, “Polymer Layered Silicate Nanocomposites: Perparation and Properties and Uses of a New Class of Materials” Mater. Sci. Eng. R Rep” 28 (2000) 1-63.
7. Okada, A and Usuki, A, “Chemistry of Polymer-Clay Hybrids”, Mater. Sci. Eng. C 3 (1995) 109-115.

### 12CH316 ADVANCED PHARMACEUTICAL CHEMISTRY

Credits 4:0:0

**Course objective:**

- To equip the students with a thorough understanding of different aspects of pharmaceutical chemistry.

**Course Outcome:**

- After finishing this course, the student will be able to understand and apply the design and synthetic approaches used in pharmaceutical chemistry.

**Unit 1**

**BASICS OF MEDICINAL CHEMISTRY:** Introduction to drug design - Physical and chemical factors associated with biological activities - Classification of drugs based on structure or pharmacological basis with examples – Pro drugs and soft drugs – Design of pro drug system – Multiple pro drug formation – Soft drug principle and applications – Quantitative Structure Activity Relationship – Chirality in Drug Design.

**Unit II**

**DRUG DISCOVERY AT THE ENZYME LEVEL:** Enzymes and enzyme inhibitors – Competitive and non-competitive inhibitors – Reversible and irreversible inhibitors – Ligand-receptor theories – Clark's theory and Paton's rate theory – Proteins, lipids, and nucleic acids as drug targets – Effect of pH, pK<sub>a</sub>, and polarity on drug solubility – DNA Protein interaction and DNA drug interaction.

**Unit III**

**DRUG ACTION AND DRUG METABOLISM:** Drug action – Ideal requirement of a drug – sources of drug plant and animal origin, synthetic and semisynthetic drug – Mechanism of Drug Action - Absorption, distribution, metabolism, and elimination – Oxidation and hydrolysis – Testing drugs in vitro – High-throughput screening – Testing drugs in vivo – Therapeutic index and therapeutic ratio.

**Unit IV**

**DEVELOPMENT OF NEW DRUGS & TYPES OF DRUGS:** Five classic steps in the design of a new drug – Procedures in drug design – Molecular modification of lead compounds – Factors affecting drug development – Analgesics – Local and General Analgesics - Classification – Mechanism of action with examples – Anesthetics – Local and General Anesthetics - Classification – Mechanism of action with examples.

**Unit V**

**VARIED CLASS OF DRUGS:** Structure, Synthesis and mechanism of action of Selected Drugs - Antibiotics – Ciprofloxacin, Norfloxacin - Antiviral agents - Idoxuridine - Acyclovir - Antipsychotics – Clozapine - Chlorpromazine - Antineoplastics - Lomustine - methotrexate – Anti HIV – Azidothymidine - Dideoxythymidine.

**Text Books**

1. Ashutosh Kar, "Medicinal Chemistry" New Age International Publishers, 5th Revised and Expanded edition, 2010.
2. Rama Rao Nandella, "Principles of Organic Medicinal Chemistry" New Age International Publishers, New Delhi, Reprint, 2005.
3. Gareth Thomas "Fundamentals of Medicinal Chemistry", London, Reprint, 2003.

## Reference Books

1. David A. Williams, William O. Foye, Thomas L. Lemke, Lippincott Williams & Wilkins, Foye's Principles of Medicinal Chemistry, Philadelphia, 5th edition, 2002.
2. Richard B. Silverman, "The Organic Chemistry of Drug Design and Drug Action", 2nd Edition, Academic Press, Reprinted, 2010.
3. Donald J. Abraham, David P. Rotella, "Burger's Medicinal Chemistry, Drug Discovery and Development, 8 Volume Set, John Wiley & Sons Ltd., 7th Edition, 2003.
4. Graham L. Patrick, "An introduction to Medicinal Chemistry", Oxford university Press, 1995.

## 12CH317 INDUSTRIAL ELECTROCHEMISTRY

Credits 4:0:0

### Course Objective:

- To know about metal finishing and synthesis of electrochemical inorganic / organic materials.
- To learn about electrochemical powder sources and solar cells.

### Course Outcome:

- Students will get exposed to underlying electrochemical principles of metal finishing, electrochemical materials, electrochemical power sources and solar cells.

### Unit I

**Metal Finishing:** Electrodeposition potential, E.m.f series, Electroplating process, Faraday's laws, Anodes for plating, Effects of plating variables, Throwing power of the bath, General principles of surface preparation - Electroplating of copper, chromium, zinc and gold - Electroplating for electronic industry- Electroless plating of nickel- Anodizing – Electroforming.

### Unit II

**Conducting Polymers and Electrochemicals:** Electropolymerisation- anodic and cathodic polymerization- Effects of reaction parameters on the course of the reaction- Electrochemical preparation of conducting polymers- Electrolytic production of perchlorates and manganese dioxide – Electroorganic synthesis of adiponitrile and hydroquinone.

### Unit III

**Batteries and Power Sources – I:** Principles of energy conservation- Electrochemical energyconservation- Thermodynamic reversibility - Gibb's equation - Classification of batteries, types of electrolytes - Battery characteristics - Battery specifications - Battery components, Evaluation of battery performance.

### Unit IV

**Batteries and Power Sources – II:** Construction and characteristics of primary batteries: Dry Leclanche cells, alkaline primary batteries and family of lithium batteries - Secondary batteries: Lead acid – car, traction, stationary, standby and sealed batteries. Nickel cadmium – pocket plates and sintered plates – vented and sealed maintenance free designs. Fuel cells- Introduction, types of fuel cells, advantages.

### Unit V

**Solar Cells: Material Science Approach:** Principles and characteristics of Solar cells, Materials approach: fabrication of pure, polycrystalline, amorphous Si cells and thin film solar cells - CdS/Cu<sub>2</sub>S cells. Photo electrochemical cells (PEC) for conversion of light energy into electrical energy - PEC cells based on GaAs.

**Text Books:**

1. Pletcher D. and Walsh F. C. "Industrial electrochemistry", Chapman and Hall, London, 1990.
2. Khun A. T. "Industrial Electrochemistry", Elsevier Publishers, 1972.
3. Wattman R. J. and Bargon, J. Can. J. Chem. 64, 76 (1986).

**Reference Books:**

1. Parthasarathy N. V. "Practical Electroplating Handbook", Prentice-Hall, Inc. New Jersey, 1989.
2. Baizer M. M. "Organic electrochemistry", Dekker Inc. New York, 1983.
3. Rifi M. R. and Frank. H. Covitz, "Introduction to Organic Chemistry", Dekkar Inc. New York, 1974.
4. Barak, M. "Electrochemical power sources", IEEE series, Peter Peregrinius Ltd, Steverage, U.K. 1980, reprinted during 1997.
5. Sodhi. G. S. "Environmental Chemistry", Narosa Publishing House Ltd, New Delhi, 2009.
6. David Linden, "Handbook of Batteries". Second edition. McGraw-Hill Inc, New York.
7. Venkatasubbiah, "Batteries", Efy Enterprises, Ltd, 1987.
8. Chopra K.L. and Das S. R. "Thin film and solar cells", Plenum Press, New York, 1983.
9. Janne Halme, "Dye-Sensitised Nanostructured and Organic Photovoltaic cells", Master's Thesis.
10. Garag H. P. and Prakash J., "Solar Energy: Fundamentals and Applications", Tata McGraw-Hill Publishing Company Ltd., New Delhi.
11. Coyle, J. D. Hill R. R. and Roberts D. R. (Eds) "A Source book in Photochemistry", Open University Press, U. K. 1982.
12. Bruno Scrosatti, "Applications of Electroactive polymers", Chapman & Hall, London, 1993.

## 12CH318 ENVIRONMENTAL ELECTROCHEMISTRY

**Credits: 4:0:0**

**Course Objective:**

- This course is aimed at providing the student a solid background on topics linking environmental issues such as environmental phenomena, environmental protection and remediation and manmade environmental damages, with electrochemical phenomena.

**Course Outcome:**

- The course will be divided into two main parts: In the first part the students will be exposed to basics in electrochemistry and the second part will be devoted to in-depth electrochemically oriented environmental issues.

### Unit I

**PRINCIPLES OF ELECTROLYTE SOLUTIONS:** Ion-solvent interactions (Born Model, Ion-Dipole model), ion-ion interactions (Debye-Huckel theory, ionic atmosphere), dielectric constant, the significance of Debye length, the significance of activity coefficient. Ion transport

in solutions: Diffusion, random walk, convection, migration under the influence of an electrical field, conductivity, equivalent conductivity; electrophoretic effect.

## **Unit II**

**REACTIONS AT THE ELECTRODE-SOLUTION INTERFACE:** The origin of surface charges, the metal –solution interface, the electrical double layer, outer and inner Helmholtz planes, the diffuse double layer, Gouy-Chapman-Stern theory for the structure of the electrical double layer, differential capacitance, ionic strength, the influence of ionic strength on the properties of the interface. Introduction to electrochemical kinetics: Electron transfer through the interface (the Butler-Volmer equations), Tafel equation, ion diffusion at the interface, the entire I-V curve, rate limiting step, special mass transfer cases at the interface.

## **Unit III**

**INTERFACIAL PHENOMENA-RELATED TOPICS:** Stability of colloidal systems - classification of colloids, significance of colloids in environmental issues, electrostatic interactions, London-Van der Waals interactions, Born interactions, depletion forces, the DLVO theory, coagulation and flocculation, influence of ionic strength and ionic charge (Schulze-Hardy rule) on stability - Electrokinetics - What happens to the interfacial charge distribution in a flowing solution?, the shear plane (significance of zeta potential), electroosmosis, streaming potential, electrophoresis, sedimentation potential, description by force-flux relation (according to irreversible thermodynamics), Helmholtz-Smoluchowski equation, measuring electrokinetic phenomena, soil remediation by electrokinetic phenomena.

## **Unit IV**

**ELECTROCHEMICAL REACTORS** - Classification of electrochemical reactors, unique features of electrochemical reactors, structure, energy consumption, space-time yield, advantages and disadvantages of electrochemical reactors, special types of electrochemical reactors.

## **Unit V**

**ENVIRONMENTALLY-RELATED ELECTROCHEMICAL ISSUES** - Electrochemical methods for water and wastewater purification- removal of metals, oxidation and reduction of organic contaminants (direct oxidation or reduction, mediated electrochemical oxidation- the CerOx process, ex-situ electrochemical production of oxidizing agents- chlorine, ozone, hydrogen peroxide, ClO<sub>2</sub>), electrodialysis –principles and applications, principles of electrochemical measurements and sensing, fuel cells and bioelectrochemistry for cleaner energy, electrocoagulation.

## **Text Books**

1. Koryta, J. Dvorak J., Kavan L. “Principles of Electrochemistry”, John Wiley Publishers, 1993.
2. Glasstone, S. Textbook of Physical Chemistry, Macmillan, Bombay, India, 2nd edition, 1974.

## **Reference Books**

1. Duncan A MacInnes, “The principles of Electrochemistry”, Reinhold publishing corporation, 1998.
2. Bockris & Reddy, “Modern Electrochemistry”, Springer, Volumes 1 & 2, 1973.

3. K Scott, "Electrochemical Reaction Engineering", Academic Press, London, 1991.
4. P. Delahay, "Double Layer and Electrode Kinetics", USA: Wiley-Interscience, 1965.
5. C. A. C. Sequeira, "Environmental oriented electrochemistry", Elsevier 1994.
6. Christos Comninellis, Marc Doyle, Jack Winnick, "Energy and electrochemical processes for a cleaner environment: proceedings" by Electrochemical Society, International Society of Electrochemistry, Electrochemical society Etats-Unis Energy technology division, Electrochemical Society Meeting. - Science – 2001.

## **12CH319 MOLECULAR AND MATERIALS SELF-ASSEMBLY**

**Credits: 4:0:0**

### **Course Objective:**

- The assembly of nanomaterials of different types will be discussed.
- The student will get knowledge on the bottom-up approach in nanotechnology based on self-assembly.
- The student will be able to distinguish molecular and materials self-assembly on the basis of the driving force needed for them to form.

### **Course Outcome:**

- Self-assembly, which is the most basic of bottom-up building up of nanostructures will be learnt in detail by the student.

### **Unit I**

#### **FUNDAMENTALS OF SELF-ASSEMBLY AND SELF-ASSEMBLED MONOLAYERS:**

Self-assembly: definition – Molecular vs. materials self-assembly – Hierarchical self-assembly – Forms, patterns and functions – Self-assembled monolayers (SAMs) – Soft lithography – Microlens arrays – Transfer printing – Electrically contacting SAMs – SAM crystal engineering – Switching SAM function – Chemical reactions on SAMs – Applications of SAMs.

### **Unit II**

**LAYER-BY-LAYER SELF ASSEMBLY:** Electrostatic superlattices – Organic polyelectrolyte multilayers – Assembling metallo-polymers – Polyelectrolyte-Colloid multilayers – Graded composition LbL films – LbL MEMS – Crystal engineering of oriented zeolite film – Zeolite-ordered multi-crystal arrays – Cross-linked crystal arrays – Patterned multilayers – Non-electrostatic LbL assembly – LbL self-limiting reactions.

### **Unit III**

**NANOROD, NANOWIRE SELF-ASSEMBLY:** Templating nanowires – Modulated diameter gold nanorods – Self-assembling nanorods – Magnetic nanorods – Magnetic nanorods and nanoclusters – Hierarchically ordered nanorods – Nanorod devices – Nanotubes from nanoporous templates – VLS synthesis of nanowires – Nanowire quantum size effects – Manipulating nanowires – Crossed semiconductor nanowire smallest LCD – Nanowire sensors.

### **Unit IV**

**NANOCLUSTER SELF-ASSEMBLY:** Definitions for nanocrystal, nanoparticle, and nanocluster – Synthesis of capped semiconductor nanoclusters – Electrons and holes in nanocluster boxes – Nanocrystal semiconductor alloys – Nanocluster phase transition – Capped

gold nanoclusters – Alkanethiolate capped nanocluster diagnostics – Water soluble nanoclusters – Alkanethiolate capped silver nanocluster superlattice – Core-shell magnetic nanoclusters – Nanocluster- Polymer nanocomposites.

### Unit V

**SELF-ASSEMBLING BLOCK COPOLYMERS:** Block copolymer self-assembly – Nanostructured ceramics – Block copolymer thin films – Electrical ordering – Spatial confinement of block copolymers – Block copolymer lithography – Decorating block copolymers – Nanowires from block copolymers – Making micelles – Harnessing rigid rods – Block co-polypeptides – Block copolymer bio-factories.

### Text Books

1. Tomorrow's chemistry today–Concepts in nanoscience, organic materials, and environmental chemistry, Bruno Pignataro, Wiley-VCH, Royal chemical society, 2008.
2. Nanochemistry, G.B. Sergeev, Elsevier, 2007.

### Reference Books

1. Nano: The essentials, T. Pradeep, McGraw Hill Publishers, 2007
2. Core Concepts on supramolecular chemistry and nanochemistry, Jonathan Steed, Wiley Eastern Publishers, 2006
3. <http://www.uaf.chem/rfk/nano.html>
4. The physics and chemistry of nanosolids, Frank J. Owens and Charles P. Poole Jr., Wiley Interscience Publishers, 2006
5. Encyclopedia of nanochemistry, R. Thomson, Anmol Publishers, 2005
6. Nanoscale technology in biological systems, Ralph G. Grew, Fritz B. Prinz, and R. Lane Smith, CRC Press, 2007
7. Nanoscale materials, Parag Diwan and Ashish Paradwaj, Pentagon Publishers, 2007

## 12CH320 CHEMICAL APPROACH TO NANOMATERIALS

**Credits: 4:0:0**

### Course Objective:

- Soft lithographic patterning on the basis of chemistry will be discussed.
- The theory of materials preparation with soft building blocks and large building blocks will be taught to the students.
- The question of how chemistry uses bioinspiration for material preparation will be addressed.

### Course Outcome:

- The student will get a thorough knowledge of the chemical approach to patterning and synthesis of nanomaterials.

### Unit I

**NANOCONTACT PRINTING:** Soft lithography – Micro-contact printing – Defect patterning – Below 50 nm nanocontact printing – Nanocontact writing – Dip-pen nanolithography (DPN) – Nanoscale writing on semiconductor nanowires – Soft patterning of hard magnets – Patterning

bio-constructions – Enzyme DPN – SPM Nano-electrochemistry – Scanning probe contact printing (SP-CP) – Nanoplotters.

### **Unit II**

**MICROSPHERES:** Photonic crystals – Microsphere building blocks – Silica microspheres – Multi-shell microspheres – Microsphere self-assembly crystals and films – Photonic crystal marbles – Photonic crystal fibers – Optical properties of colloidal crystals – Synthesizing photonic band gap – Internal light sources – Photonic inks – Color oscillator – Photonic crystal sensors - Liquid crystal photonic crystal.

### **Unit III**

**POROUS MATERIALS FROM SOFT BUILDING BLOCKS:** Modular self-assembly of microporous materials – Hydrogen storage coordination frameworks – Microporous materials – Mesoscale building blocks – Designing function into mesoporous materials – Mesostucture and dimensionality – Mesotexture – Silica-polymer hybrids – Guests in mesopores – Organics in the backbone – Films, interfaces, mesoepitaxy – Mesomorphology.

### **Unit IV**

**LARGE BUILDING BLOCKS:** Supra-micron shapes assembly – Crystallizing micron-sized planar building blocks – Polyhedra with patterned faces – Large sphere building block assembly – Magnetic self-assembly – Dynamic self-assembly – Autonomous assembly – Synthetic life – Large sphere building blocks and 3D crystals.

### **Unit V**

**BIOMATERIALS AND BIOINSPIRATION:** Nature's design of materials – Mimicking nature – Faux fossils – Siliceous sculptures – Synthetic morphology – Biomimicry – Biomineralization – Learning from nature – Viral cage directed synthesis of nanoclusters – Polynucleotide directed nanoclusters – DNA coded nanoclusters – Bacteria directed materials self-assembly – Protein S-layers – Better bones through chemistry.

### **Text Books**

1. Bruno Pignataro, Tomorrow's chemistry today–Concepts in nanoscience, organic materials, and environmental chemistry, Wiley-VCH, Royal chemical society, 2008.
2. Sergeyev G.B., Nanochemistry, Elsevier, 2007.

### **Reference Books**

1. Pradeep T., Nano: The essentials, McGraw Hill Publishers, 2007.
2. Steed, Jonathan, Core Concepts on supramolecular chemistry and nanochemistry, John Wiley Publishers, 2006.
3. Owens, Frank J. and Poole Jr. Charles P., The physics and chemistry of nanosolids, Wiley Interscience Publishers, 2006.
4. Thomson R., Encyclopedia of nanochemistry, Anmol Publishers, 2005.
5. Grew, Ralph G., Prinz, Fritz B., and Smith, R. Lane, Nanoscale technology in biological systems, CRC Press, 2007.
6. Parag Diwan and Ashish Paradwaj, Nanoscale materials, Pentagon Publishers, 2007.

## **12CH321 MOLECULAR MACHINES AND MATERIALS**

**Credits: 4:0:0**

### **Course Objective:**

- Structure, function and classifications of specific nanomaterials will be discussed.
- Distinguishing element-based function of nanostructures will be known to the students.
- The student will know how these nano-sized materials work strange in suitable conditions.

### **Course Outcome:**

- The applications of nanostructures in various fields, based on the structure and function of molecular machines, carbon nanostructures, and dendrimers, will be taught to the students.

### **Unit I**

**MOLECULAR MACHINES:** Historical basis for molecular machines – Molecular nanotechnology - Molecular motors: examples, modern insights – Smart materials and nanosensors – Replicating nanorobots – Molecular propeller – Molecular switches, rectifiers, wires – Molecular shuttle – Molecular tweezers – Molecular logic gates – Molecular assembler – Drexler and Smalley debate.

### **Unit II**

**FULLERENES, GRAPHENES:** Allotropes of carbon – Diamond and graphite; Fullerenes: nomenclature, bucky-balls, carbon nanobuds, solubility, safety and toxicity, fullerites, chemical properties of fullerenes, fullerene reactions – Fullerenes as ligands – Fullerene synthesis – Graphenes – Hybridization in graphenes – Epitaxial growth on silicon carbide – Epitaxial growth on metal substrates – Properties –Electronic properties – Thermal properties – Mechanical properties – Potential applications.

### **Unit III**

**DENDRIMERS:** Introduction –General structure – Synthesis – Click chemistry – Classification as linear, cross-linked, branched, and dendritic polymers - Properties and applications – Types of dendrimers as PAMAM, PAMAMOS, PPI, and Tacto dendrimers – Frechet type dendrimers – Chiral dendrimers – Divergent dendrimer growth – Convergent dendrimer growth – Mixed growth.

### **Unit IV**

**NANOTUBES:** Nanotubes: carbon nanotubes – Classification as single walled and multi walled – Kinetic, thermal, and electrical properties – Defects – Synthesis of nanotubes – Structural, electro-acoustic, electromagnetic applications of nanotubes – Nanotubes in electrical circuits – Selective chemistry of single-walled nanotubes.

### **Unit V**

**QUANTUM DOTS CHEMISTRY:** Quantum dots, quantum wires and wells – Making quantum dots – Colloidal synthesis – Fabrication – Viral assembly – Electrochemical assembly – Optical properties – Applications in biology and computing – Applications in photovoltaic devices and light emitting devices.

### **Text Books**

1. Owens, Frank J. and Poole Jr. Charles P., The physics and chemistry of nanosolids, Wiley Interscience Publishers, 2006.
2. Brechignac C., Houdy P., Lahmani M., Nanomaterials and nanochemistry, Springer, 2006.

### **Reference Books**

1. Cantor, Brian, Novel nanocrystalline alloys and magnetic nanomaterials: An Oxford–Kobe materials text, IoP publishing ltd., 2005.
2. Miller J.C., Serrato R.M., Cardenas J.M.R., Kundahl G.A., The handbook of nanotechnology, John Wiley & sons, 2005.
3. Rao, C.N.R., Cheetham A.K., Materials science at the nanoscale Taylor & Francis group, 2006.

## **12CH322 NANOTECHNOLOGY IN FUEL CELLS AND ENERGY STORAGE**

**Credits: 4:0:0**

### **Course Objective:**

- The application of nanotechnology in energy storage will be discussed.
- The question of possibility of alternative energy will be met with on theoretical basis.
- The materials in use for such energy storage will be introduced to the students.

### **Course Outcome:**

- The student gets an exposure to the role of nanotechnology in meeting the energy needs of the future.

### **Unit I**

#### **NANOSTRUCTURED CATALYSTS FOR LOW TEMPERATURE FUEL CELLS:**

Working principle of a fuel cell – Electrode reactions at low temperature fuel cells – Supported catalysts – Catalyst preparation – Impregnation method, colloidal method, micro-emulsion method – Catalyst supports – Nanostructured carbon – Nanoporous carbon – Mesoporous carbon – Hierarchical pore structures.

### **Unit II**

**NANOCRYSTALLINE SOLAR CELLS:** Dye-sensitized solar cells – Cell operation, materials – Semiconductor-sensitized solar cells (SSSC) – Liquid junction SSSCs – Recombination rates in semiconductors – Back-transport of electrons from oxide to absorbing semiconductor – Electron injection from oxide / substrate into electrolyte.

### **Unit III**

**OXIDES AND SOLID-STATE SSSCS:** Losses in semiconductor aggregates on oxides – Multilayer semiconductors – Other porous oxides – Solid state semiconductor-Sensitized solar cells (sSSSCs) – The ETA cell – Two-component ETA cells - Three-component ETA cells – Built-in fields in SSSCs.

### **Unit IV**

## **NANO-SCALE MATERIALS FOR HYDROGEN AND ENERGY STORAGE:**

Introduction – Methods for energy storage – Energy storage in super-capacitors and batteries – Hydrogen storage in mobile applications – Challenges in material development – Physisorption materials – Nanoporous inorganic materials for hydrogen storage – Zeolite-based and transition metal-based structures.

### **Unit V**

**NANO-POROUS ORGANIC MATERIALS FOR HYDROGEN STORAGE:** Nanoporous organic and carbon materials – Activated carbon, carbon nanotubes, carbide-derived carbons – Metal-organic framework – Chemisorption materials – Magnesium hydride, complex hydrides – Reaction systems – Experimental aspects – Materials handling – Synthesis methods – Characterization of hydrogen storage materials – Thermodynamic and kinetic properties of hydride systems.

### **Text Books**

1. Wilde, Gerard Nanostructured materials, Elsevier, 2009.
2. Hart A.B. and Womack G. J., “Fuel Cells: Theory & Applications”, Prentice Hall, NY.
3. Narayan R and Viswanathan B, “Chemical and Electrochemical Energy Systems”, University press (India) Ltd., 1998.

### **Reference Books**

1. Nanotechnology: clean energy resources for the future, Gillett, Stephen L., Foresight institute, 2002.
2. Holladay, Jamelyn D., Wang, Yong, Jones, Evan. Chemical Reviews 2004, 104, 4767 – 4790,

## LIST OF SUBJECT

| Code    | Subject Name      | Credits |
|---------|-------------------|---------|
| 13CH201 | Applied Chemistry | 3:0:0   |

### 13CH201 APPLIED CHEMISTRY

**Credits: 3:0:0**

**Objective:**

- To understand industrial and domestic problems associated with water and learn about treatment methods.
- To learn the properties and uses of industrially important polymers and bio-polymers.
- To understand the fuel chemistry and its importance in our daily walk of life.
- To have an understanding about different energy sources such as batteries, fuel cell etc.
- To impart the basic concepts of materials used in engineering.

**Outcome:**

- To suggest methods to minimize problems related to hard water in industrial operations.
- To select and use eco-friendly fuels, polymers and engineering materials for industrial and domestic purpose.
- To use appropriate methods to minimize corrosion of metals.

**Unit I**

**WATER TECHNOLOGY:** Sources of water-hardness of water-units of hardness-estimation of hardness-EDTA method and alkalinity method-softening of hard water- Zeolite process-demineralization or ion-exchange process-scale and sludge formation in boilers-internal conditioning-colloidal, phosphate, calgon, carbonate, complexometric conditioning, boiler corrosion-caustic embrittlement - desalination - electro dialysis, reverse osmosis, water for drinking purpose.

**Unit II**

**HIGH POLYMERS:** Nomenclature- Tacticity- Functionality- Classification based on structure, synthesis and molecular forces-Types of Polymerisation-addition, condensation, copolymerisation- Plastics- moulding constituents of plastics- foamed plastics, fibre-reinforced plastics- Preparation, properties and uses of polyethylene (PE) -polyvinyl chloride (PVC)-phenolic resin -nylons-epoxy resin- Rubber - vulcanization of rubber, Biopolymers – Carbohydrates and Proteins – (definition and uses only).

**Unit III**

**FUELS AND COMBUSTION:** Fuels – classification, Combustion - Gross and Net Calorific values (Dulong's formula) - calculation of air quantities - simple problems - Flue gas analysis-Orsat's apparatus – Solid fuels – Coal-Proximate analysis and Ultimate analysis - significance-Metallurgical coke – carbonisation (definition) -characteristics of metallurgical coke-Liquid fuels

-synthetic petrol-cracking (definition)-Knocking-Octane number -improvement of anti-knocking characteristics, Diesel engine fuels-Cetane number, Gaseous fuels-Manufacture of water gas - CNG, LPG –definition, Biogas- Manufacture of Gobar gas (fixed dome type), Rocket propellant – types.

#### **Unit IV**

**ELECTROCHEMISTRY:** Electrode potential-measurement of electrode potential-Nernst equation for electrode potential-electrochemical series-electrochemical cell or Voltaic cell-Concentration cell-Primary cell-Leclanche cell-Secondary batteries- lead acid battery – Fuel cell – H<sub>2</sub>-O<sub>2</sub> cell – Corrosion -types – Chemical corrosion – oxidation corrosion, corrosion by other gases, electrochemical corrosion- types – galvanic corrosion, concentration cell corrosion - Factors influencing corrosion-Corrosion control methods.

#### **Unit V**

**ENGINEERING MATERIALS:** Refractories – classification – requisite properties - manufacturing steps- common refractories -silica bricks, dolomite bricks - Insulators – characteristics – electrical insulating materials – thermal insulators – classification - properties – Lubricants – Friction and wear, functions of lubricant – classification of lubricants – lubricating oils – semi solid lubricants – solid lubricants – selection of lubricants.

#### **Text books**

1. Jain P. C, Monica Jain, “A text book of engineering chemistry”, Dhanapat Rai publications, New Delhi, 12th edition, 2006.

#### **Reference Books**

1. Gowarikar V. R, Viswanathan N. V, Jaydev Sreedhar, “Polymer Science”, New Age International Pvt. Ltd., New Delhi, 2000.
2. Agarwal C. V, “Chemistry of Engineering materials”, C.V. Tara Book Agency, 1982.
3. Shashi Chawla, “A text book of engineering chemistry”, Dhanapat Rai publications, New Delhi, 8th edition, 2008.
4. Subha Ramesh, Vairam, Anandhan, “Engineering Chemistry”, Wiley India Pvt. Ltd., New Delhi, 2011.