### DEPARTMENT OF CHEMISTRY

**BHARATHIAR UNIVERSITY: COIMBATORE – 641 046.**

**M.Sc. Chemistry – 2017-2018 onwards**

Under choice based credit system (CBCS)

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As per the CBCS, each PG student is allowed to choose 3 supportive courses offered by the other departments of the university.
Subject Title: ORGANIC CHEMISTRY – I (Reaction Mechanisms)

Course Code: CHMA13A Number of credit hours: 4 (four)

Subject Description:

This course presents the principles of various organic reactions and outlines the mechanism and discusses the applications of reactions.

Goals:

To enable the students to learn the principles of reaction mechanism and modern reagents used for various reactions.

Objectives

On successful completion of the course the students should have

i) Understood the principles and reaction mechanism involving various electrophonic, nucleophilic, addition, elimination, redox reactions & molecular rearrangements:

Contents

Unit – I

Aliphatic and Aromatic Nucleophilic Substitution Reactions:

Bonding - structure and reactivity - acids and bases (hard and soft acid base theory) - methods of determination and the study of reaction mechanisms.

$S_N^1$, $S_N^2$, $S_N^i$ and neighbouring group mechanisms - kinetics - effects of structure - solvent and leaving and entering group - stereochemistry - hydrolysis of esters - Wurtz reaction - Claisen and Dieckmann condensation - Williamson reactions.

Different mechanisms of aromatic nucleophilic substitution - Ziegler alkylation - Chichibabin reaction - cine substitution - diazonium group as leaving group.
Unit - II

Aliphatic and Aromatic Electrophilic Substitution Reactions:

$S_E^1$ and $S_E^2$ reactions - mechanisms and reactivity - typical reactions involving migration of double bond - keto-enol tautomerism - halogenation of carbonyl compounds - Stork enamine reactions - decarboxylation of aliphatic acids - Friedel Crafts acylation of olefinic carbon.

Aromatic electrophilic substitution - reactivity - orientation and mechanisms - nitration - halogenation and sulphonation - Friedel Crafts alkylation - Friedel Crafts arylation (Scholl reaction) and acylation - Jacobsen reaction - formylation with (i) disubstituted formamides(Vilsmeier-Haack reaction) (ii) zinc cyanide and HCl (Gattermann reaction) (iii) chloroform (Reimer-Tiemann reaction) - carboxylation with (i) carbonyl halides (ii) carbon dioxide (Kolbe Schmidt reaction) - amidation with isocyanates - hydroxyalkylation (hydroxyalkyl - dehydrogenation)- cyanodehydration of aldehydes and ketones (Bradsher reaction and Bischler-Napieralski reaction) - haloalkylation - aminoalkylation and amidoalkylation - thioalkylation -acylation with nitriles (Hoesch reaction) - cyanation - hydroxylation.

Unit – III
Molecular Rearrangements:


Unit – IV

Addition and Elimination Reactions:

Addition to C-C and C-O multiple bonds - electrophilic, nucleophilic and free-radical additions - additions to conjugated systems - orientation - Birch reduction - hydroboration -
Michael condensation - 1,3 dipolar additions - Diels-Alder reactions - carbene addition to double bonds - hydration of olefines.


Unit - V

Oxidation and Reduction:

Formation of C=C, C-C bonds by dehydrogenation - dehydrogenation by quinones, SeO₂, Hg(OAc)₂, and Pb(OAc)₂. formation of C-C bond in phenol coupling - acetylene coupling - allylic oxidation - oxidation of alcohols, glycols, halides and amines to aldehydes and ketones - ozonolysis - oxidation of olefinic double bonds and unsaturated carbonyl compounds - oxidative cleavage of the C-C bond - Sommelet reaction and selectivity in reduction - metal hydride reduction - metal alkoxide reduction - reduction by dissolving metals - Clemmensen reduction - Wolf Kishner reduction - metal ammonia reduction (Birch reduction) - reduction of nitro compounds - acyloin condensation - catenanes.

Carbenes and nitrenes - structure and generation - addition reaction with alkenes - insertion reactions.

References
Subject Title: INORGANIC CHEMISTRY – I (Coordination Chemistry)

Course Code: CHMA13B

Number of credit hours: 4(four)

Subject Description:
This course presents the basic theories of coordination compounds, structure of different complexes with varying coordination numbers and a study of magnetic and electronic properties. New cluster compounds and their structures are also discussed.

Goals:
To motivate the students to understand the basic principles of coordination chemistry

Objectives:
On successful completion of the course the students should have

i) Learnt about the various theories of complexes, mode of coordination with various geometry.

ii) Studied the recent development in polymeric materials of coordination complexes

Contents

Unit - I

18 electron rule - EAN rule - theories of coordination compounds - valence bond theory - crystal field theory - splitting of d orbitals in different symmetries - crystal field stabilization energy - factors affecting the magnitude of 10 Dq - evidence for crystal field stabilization - spectrochemical series - site selection in spinels - tetragonal distortion from octahedral symmetry - Jahn-Teller distortion - molecular orbital theory - octahedral complexes - tetrahedral and square planar complexes - pi bonding and molecular orbital theory - experimental evidence for pi bonding.

Unit - II

Term states of d^n ions - electronic spectra of coordination compounds - selection rules - band intensities and band widths - energy level diagrams of Orgel and Tanabe - Sugano - spectra of Ti^{3+}, V^{3+}, Ni^{2+}, Cr^{3+}, Co^{2+}, Cr^{2+} and Fe^{2+} - calculation of 10Dq and B for V^{3+}_{(oct)} and Ni^{2+}_{(oct)} complexes.
Magnetic properties of coordination compounds - change in magnetic properties of complexes in terms of spin orbit coupling - temperature independent paramagnetism - spin cross over phenomena.

Unit - III

Substitution reactions in square planar complexes - the rate law for nucleophilic substitution in a square planar complex - the trans effect - theories of trans effect - mechanism of nucleophilic substitution in square planar complexes - kinetics of octahedral substitution - ligand field effects and reaction rates - mechanism of substitution in octahedral complexes - reaction rates influenced by acid and bases - racemisation and isomerisation - mechanisms of redox reactions - outer sphere mechanisms - excited state outer sphere electron transfer reactions - inner sphere mechanisms - mixed valent complexes.

Unit - IV

Structure of coordination compounds with reference to the existence of various coordination numbers - complexes with coordination number two - complexes with coordination number three - complexes with coordination number four - tetrahedral and square planar complexes - complexes with coordination number five - regular trigonal bipyramidal and square pyramidal - site preference in trigonal bipyramidal complexes - site preference in square planar complexes - isomerism in five coordinate complexes - coordination number six - distortion from perfect octahedral symmetry - trigonal prism - geometrical isomerism in octahedral complexes - coordination number seven and eight.

Unit - V


References

1. Inorganic Chemistry - Principles of structure and reactivity, Fourth Edition
CORE III

Subject Title: PHYSICAL CHEMISTRY – I (Electrochemistry & Photochemistry)

Course Code: CHMA13C       Number of credit hours: 4(four)

Subject Description:
This course presents the basic principles of electrochemistry, photochemistry and nanotechnology with respect to their applications.

Goals:
To enable the student to learn the theories and basics of electrochemistry, photochemistry and various applications of electrochemical/photochemical and nanotechnological approaches.

Objectives:
On successful completion of the course the students should have learnt about the fundamentals of electrochemistry, photochemistry and importance of nanotechnology.

Contents

Unit – I ELECTROCHEMISTRY - I

Ions in solutions:

Unit – II  ELECTROCHEMISTRY - II

Metal/Electrolyte interface:


Unit – III  ELECTROCHEMISTRY - III

Electrochemical cells:

Electromotive force - measurement of EMF - the potentiometer - the electrochemical potential - the cell EMF and the cell reaction - reversible cells - types of half cells - classification of cells - the standard EMF of a cell - standard electrode potentials - calculation of the EMF of a cell - Nernst equation and its limitations - calculation of solubility products - standard free energies and entropies of aqueous ions - electrode concentration cells - electrolyte concentration cells - cells with liquid junctions - oxidation - reduction reactions, measurement of pH, concentration cells with transference – Electrochemical energy systems - Li-ion batteries-Methanol Fuel cells.

Unit – IV  PHOTOCHEMISTRY

Unit – V  COLLOIDS AND CHEMISTRY IN NANOSCIENCE & NANOTACHNOLOGY


References

ELECTIVE-I

Subject Title: PHYSICAL METHODS IN CHEMISTRY

(Molecular spectroscopy and Surface morphological studies)

Course Code: CHMA1EA Number of credit hours: 4(four)

Subject Description:

This course presents the basic principles of molecular spectroscopy

Goals:

To motivate the students to understand the basic principles of molecular spectroscopy

Objectives:

On successful completion of the course the students should learn the principles involved in molecular spectroscopy.

Contents

Unit – I ROTATIONAL SPECTROSCOPY


Unit – II VIBRATIONAL SPECTROSCOPY

Unit – III

Raman Spectroscopy:

Pure rotational Raman spectra – Vibrational Raman spectra – selection rule - Polarization of light and the Raman effect – Structural determination from Raman spectroscopy – Techniques and Instrumentation.

Electronics spectroscopy of atoms:


Unit – IV  ULTRAVIOLET AND VISIBLE SPECTROSCOPY


Unit – V  RADIATION CHEMISTRY AND MORPHOLOGICAL STUDIES:


Introduction to Surface characterization methods – AFM, SEM, FE-SEM, HR-TEM, STEM - Sample preparation of characterization only.

References

2. Chang - Basic principles of spectroscopy.
ELECTIVE II

Subject Title : WATER TREATMENT, FUELS AND POLYMERS
Course Code : CHMA1EB Number of credit Hours: 3 (Three)

Subject Description: This paper deals with the Water Chemistry (water treatment, conditioning etc.,), Fuel chemistry (types, new sources of fuels suitable for modern world), Environmental Chemistry (Causes & Prevention) and Polymer Chemistry (polymers in life).

Goal:

1. To teach the students the essential role of water in industries and to preserve the same.

2. To teach the importance of various types of fuels and their applications.

3. To create awareness on environmental pollution.

4. To impart the knowledge on the chemistry of polymers and their crucial applications.

Unit I: Water Treatment

Sources of water – Molecular structure and physical properties – Hydrogen Bonding – Water as a solvent – Quality characteristics of water: total acidity and alkalinity, hardness of water – methods of determination of hardness, total solids, disadvantages of using hard water - Comparative account on physical and chemical properties of H₂O and D₂O.

Unit II: Water conditioning

Softening of water: Desalination, Clark’s process, lime-soda process, ion-exchange process; demineralization of water - Treatment of water: sterilization, flocculation, Industrial treatment – Treatment of wastes or effluents with organic and inorganic impurities, sewage and sewage treatment; Biochemical oxygen demand (BOD), chemical oxygen demand (COD)
Unit III: Fuels


Unit IV: Environmental Pollution

Components of environment – Factors affecting environment - Environmental pollution – Definition, pollutants, classification of pollutants - Types of pollution: air, water soil, thermal, radioactive and noise pollutions - Prevention and control of pollutions

Unit V: Plastics (High Polymers)

Introduction, classification, difference between thermosetting and thermoplastics- Effect of polymer structure on properties - Formation of plastics : copolymerization, difference between addition and condensation polymerization – Properties and uses of plastics – Moulding of plastics - Commercial resins and plastics: bakelite, urea-formaldehyde, melamine-formaldehyde, epoxy, acrylic and silicon resins, polythene, PVA, PVC, cellulose, cellulose nitrate and acetate- Disposing of plastics : incineration, biodegradation, recycling and source reduction.

Books recommended

1. Industrial Chemistry (Including Chemical Engineering) -- B.K.Sharma (10th Edition, 1999)
CORE PRACTICALS

Subject Title: ORGANIC PRACTICALS

Course Code: CHMA13P Number of credit hours: 4(four)

Subject Description:

This practical deals about the quantitative and qualitative analyses and preparation of organic compounds by standard organic reactions.

Goals:

To motivate the students to understand the basic principles of lab techniques adopted in organic laboratories

Objectives:

On successful completion of the course the students should have

i) Learnt about the quantitative and qualitative analyses by separation.
ii) Learnt the preparation of organic compounds

Contents

1. Qualitative analysis:
   Analysis of two component mixtures - separation and characterisation of the components.

2. Quantitative analysis:
   Estimation of phenol, aniline, ketone and reducing sugars - estimation of functional groups like hydroxyl, methoxyl, carbonyl and nitro groups.

3. Single stage preparation:
   Preparation of about eight organic compounds by single stage.

   (i) Benzoic acid from ethyl benzoate
   (ii) Acetanilide from aniline
   (iii) Acetylsalicylic acid from salicylic acid
   (iv) 2,4,6-Tribromoaniline from aniline
   (v) p-Bromoacacetanilide from acetanilide
   (vi) m-Dinitro benzene from nirobenzene
   (vii) Picric acid from phenol
   (viii) 2-Naphthylbenzoate from 2-naphthol.
SUPPORTIVE – I

Subject Title: CHEMISTRY IN CONTEXT

(Chemistry applicable to the society)

Course Code: GS06 Number of credit hours: 2(two)

Subject Description: This supportive paper deals with the basic chemistry in day-to-day life

Goals: To enable the student to understand about the ecological systems

Objectives: After completion of the course the students should have understood the effects of air and water to the society, various energy sources and polymers etc.

Contents

Unit - I

Air- Introduction- Definition- Composition of air- Air pollution-Definition-Air pollutants-Types of Air pollution - Causes of Air pollution on human health-Prevention of Air pollution.

Unit - II

Water-Introduction-Definition-Sources of water-Types of water-Water quality parameters-Water pollution- Definition-Types of Water pollution- Causes of Water pollution on human health-Prevention of Water pollution.

Unit – III

Energy - Introduction- Definition-Sources of energy- Types of energy- Renewable energy sources- Non-renewable energy sources- Nuclear energy-Applications.

Unit - IV

CORE IV

Subject Title: ORGANIC CHEMISTRY-II
(Natural Products, Proteins, Stereochemistry and Heterocyclic Compounds)

Course Code: CHMA23A Number of credit hours: 4(four)

Subject Description:
This course presents the comprehensive chemistry of natural products, terpenoids, proteins and stereochemistry.

Goals:
To enable the students to learn the synthesis and the isolation of natural products and heterocyclic compounds.

Objectives:
On successful completion of the course the students should have

i) Versatile knowledge about the isolation, heterocyclic compounds synthesis, bio-synthesis and elucidation of various natural products

ii) Understood conformational analysis and stereochemistry

Contents

Unit – I Terpenoids:
Isolation and classification - general methods to elucidate the structure of terpenoids - methods of structure elucidation and synthesis as applied to zingiberine - eudesmol - caryophyllene - abietic acid - santonin - biosynthesis of terpenes.

Unit – II Amino Acids and Proteins:
Unit - III

Conformational Analysis and Stereochemistry:


Unit - IV

Vitamins:

Structure and synthesis of vitamin B complex : vitamin B₁ (anearun) - vitamin B₂ (riboflavin) - pantothenic acid - folic acid - vitamin H (biotin) - vitamin B₆ (pyridoxine) - vitamin B₁₂ (cyanocobalamin) structure only - vitamin E (Alpha - tocopherol) - vitamin K₁ (phylloquinone) and vitamin K₂.

Unit - V

Heterocyclic Compounds:

Structure - synthesis and reactions of the following systems

a) Small ring Heterocycles - Three membered and four membered Heterocycles- aziridines, oxiranes, thiranes, azetidines, oxatanes and thietanes.


References

1. I. L. Finar, Organic chemistry, vol. I and vol. II.
Subject Title: **Inorganic Chemistry- II** (Bio-inorganic Chemistry)  
(Metals in biology and medicine)

Course Code : **CHMA23B**  
Number of Credits : 4 (Four)

Subject Description:
This course furnishes the basic knowledge about the role of metal ions both in biological systems and medicine.

Goals:
To equip the students to gain deeper knowledge about the structure-function correlation of metalloenzymes, function of metal ion(s) in the field of bioinorganic chemistry and therapy.

Objectives:
- To understand the role of various elements in the living systems.
- To acquire basic knowledge about the structure and functions of certain metallo-enzymes.
- To get an insight on the use of several spectroscopic and analytical techniques for structural investigation of bioinorganic compounds.
- To know about the mechanism of binding interactions of metal complexes with biomolecules and metal based drug action.

Unit-I
Metals and Non-metals in biological systems - Essential and trace elements - Role of different metal ions in biological systems - Sodium-Potassium pump - Ferritin - Transferrin-Blue copper proteins - Catecholase - Photosynthesis: Chlorophyll - Photosystem-I (PS-I) & II (PS-II) - Structure-function relationship.

Unit - II
Metalloenzymes - Definition - Examples - Active site structure and mechanism of action of - Carboxy peptidase-A and Carbonic anhydrase - Structure and function of Superoxide dismutase (SOD) (Fe-SOD, Mn-SOD, Cu-Zn couple SOD ad Ni SOD) and catalase enzymes - Xanthine oxidase - Nitrogenase
Unit - III

Phorphyrin system - Structure and functions of Hemoglobin and Myoglobin - Dioxygen binding, transport and utilization - Hemocyanin - Hemerythrin - Synthetic oxygen carriers - Vitamin B₁₂ co-enzyme - Non-heme iron-sulphur proteins - Ferridoxins - Rubredoxins - Cytochromes.

Unit - IV

Binding of metal ions and complexes to biomolecules, Types of binding - Nucleic acid structures - Fundamental interactions with nucleic acids - Binding interactions of tris-phenanthroline metal complexes with DNA - Techniques to monitor binding (Electronic absorption, Fluorescence and Circular dichroic spectral techniques, electrochemical behaviour, viscosity measurement and ploarimetry).

Chemotherapy - Radio diagnostic agents - MRI scanning - Chelating Agents (with special reference to EDTA) and therapy based on in vivo chelation of radio nucleotides - Dosage and toxicity.

Unit - V

Drug discovery and design - Therapeutic index and chemotherapeutic index - Structure - activity relationship - Factors governing drug design - Computer aided drug design - Bleomycin – Doxorubicin - Cancer chemotherapy - Bioinorganic chemistry of platinum and ruthenium anticancer drugs - Mechanism of action of cisplatin - Clinical trials and their significance - Applications of Coordination complexes in medicine.

References:

2. Dr Asim R Dass, Bioinorganic Chemistry 2007, Books and Allied (P) Limited.
4. Keith F. Purcell, John C. Kotz, Inorganic Chemistry
**CORE VI**

**Subject title**: PHYSICAL CHEMISTRY – II  
(Quantum Chemistry and Group Theory)

**Course Code.** CHMA23C  
**Number of credit hours:** 4(four)

**Subject Description:**

This course presents the basic principles of quantum mechanics and group theory.

**Goals:**

To enable the student to learn the theories of quantum mechanical treatment and basics of group theoretical approach.

**Objectives:**

On successful completion of the course the students should have learnt the knowledge of quantum chemistry and group theory.

**Contents**

**Unit – I** QUANTUM CHEMISTRY-I

Failure of classical mechanics and the success of quantum theory in explaining black body radiation - photoelectric effect and the H-atom spectrum - DeBroglie’s matter waves - Heisenberg’s uncertainty principle - Schrodinger equation - Born’s interpretation of the wave function - requirements of the acceptable wave function.

Algebra of operators - sums and products of operators - commutator - linear operators - eigen functions and eigen values - correspondence between physical quantities in classical mechanics and operators in quantum mechanics - Hamiltonian operator - quantisation of angular momentum and its spatial orientation - average (expectation) values - postulates of quantum mechanics.

**Unit – II** QUANTUM CHEMISTRY-II

Particle in a one dimensional box - quantisation of energy - normalisation of wave function - orthogonality of the particle in a one-dimensional box wave functions - average position and average momentum of a particle in a one-dimensional box - illustration of the uncertainty principle and correspondence principle with reference to the particle in a one-dimensional box - particle in a three-dimensional box - separation of variables - degeneracy.
Schrodinger equation for simple harmonic oscillator of a diatomic molecule - illustration of the uncertainty principle and correspondence principle with reference to harmonic oscillator. Schrodinger equation for a rigid rotor of a diatomic molecule. Schrodinger equation for the H-atom (or H-like species) - separation of variables - energy levels - radial factors of the H-atom wave functions

Unit III APPLICATIONS OF QUANTUM CHEMISTRY

Need for approximation methods - the perturbation theory (first order only) application of the perturbation method to He-atom - the variation method - applications of variation method to He-atom.


Unit IV GROUP THEORY


Groups and their properties - molecular point groups and classification - matrices-matrix representation of symmetry operations

Classes - representations - reducible and irreducible representations - properties of irreducible representations - Statement and proof of Great Orthogonality theorem and its consequences - Construction of character table for C_{2v} and C_{3v} point groups.

Unit V APPLICATIONS OF GROUP THEORY

Standard reduction formula relating reducible and irreducible representations - Symmetries of normal modes of vibration in non-linear molecules (H_{2}O, 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 ethylene and butadiene.

References
5. A. K. Chandra - Introductory quantum chemistry.
ELECTIVE III

Subject Title: INORGANIC SPECTROSCOPY
(Structural elucidation of (Bio)Inorganic compounds)

Course Code: CHMA2EA  Number of Credits: 3 (Three)

Subject Description:
This course presents the principle and applications of various spectral methods in structural determination of (bio)-inorganic compounds.

Goals:
The ultimate aim of the course is to understand the importance of various spectral methods in structural elucidation of inorganic compounds and metallo-proteins

Objectives:
- To understand the role of spectroscopic methods in inorganic chemistry.
- To acquire basic knowledge about the application of spectral methods in structural elucidation of inorganic compounds.
- To get an insight on the use of several spectroscopic and analytical techniques for structural investigation of (bio)inorganic compounds.

Unit- I - IR, Raman, ORD & CD spectroscopy

Infrared and (Resonance) Raman and spectra of metal complexes. - Molecular vibrations of di and triatomic molecules - Metal-ligand vibration - Band assignment - Resonance enhancement - Mechanisms - Excitation profiles, Multimode effect - Application to 2Fe-2S, 4Fe-4S and 3Fe-4S proteins and elucidation of binding mode of dioxygen in enzymes.

Circular Dichroism spectroscopy - Basic principle - Origin of optical activity - Chirality and nomenclature of chiral complexes - Cotton effect - optical isomerism in octahedral complexes - absolute configuration of complexes - stereoselectivity and conformation of chelate rings - Optical Rotatory Dispersion and linear dichroism - Examples - Magnetic circular dichroism theory - Determination of electronic ground state properties: saturation curves,
temperature dependence in the linear limit. Application of CD in conformation analysis of biomolecule(s) (DNA).

**Unit-II- Electron Paramagnetic Resonance and Photo-electron spectroscopy**


**Unit-IV - Inorganic NMR, NQR spectroscopy**

$^{31}$P, $^{19}$F NMR spectrum of HPX$_2$, P$_4$S$_3$, TiF$_4$, BrF$_5$, SF$_4$, SF$_6$, XeF$_4$O, C SIF$_6$, B$_3$H$_8$, NF$_3$, P$_3$N$_3$Cl$_4$F$_2$, ClF$_5$, ClF$_3$ Phosphorous and Hypophosphorous acid systems, HP(O)F$_2$, HOP(O)FH - use of lanthanide compounds as shift reagents. Applications to metalloproteins - paramagnetic complexes.

NQR - Principles – Introduction - Nuclear Quadrupole Energy Levels - Energy Levels and transition frequencies – Effect of a magnetic field - The Zeeman effect - Factors affecting the line width - Solid State Effects. Applications of NQR: Bonding in Boron trichloride and its adducts – Calculation of percentage of ionic character of a bond -

**Unit V - Mössbauer Spectroscopy**

Introduction - Principle of the Mössbauer Effect and Basic Concepts of Mössbauer Spectroscopy - Doppler shift - Experimental Resonance Conditions - Sharpness of resonance - Recoil Effect - Cross-section for Resonant Absorption - Comparison Between Electronic and Nuclear Transitions - Mössbauer-Experiment (Mössbauer spectrometer black diagram only) - Hyperfine Interactions and Mössbauer parameters: Isomer Shift, Electric Quadrupole Splitting, Magnetic Dipole Splitting, Applications: Mössbauer spectra of high- and low-spin iron compounds and tin halides systems: Prussian blue-Turn bulls blue, iron-carbonyl compounds,
Sodium nitroprusside, FeX₂, SnX₄, SnX₆, SnX₅Y (X & Y = F⁻, Cl⁻, Br⁻, I⁻) Tin halides - Spin Crossover, Molecular magnetism - Bioinorganic Compounds.

**Unit V – Photoelectron spectroscopy & X-ray Absorption spectroscopy**

Photoelectron spectroscopy (UV and X-ray) – Physical principle – Experimental details - Koopman’s theorem - chemical shift and correlation with electronic charges – Applications of PES.


**References**

1. Lawrence Que, Jr, Physical Methods in Bioinorganic Chemistry
2. Russell S Drago, Physical methods in Inorganic Chemistry
5. E. I. Solomon and A. B. P. Lever, Inorganic Electronic Structure and Spectroscopy
ELECTIVE IV

Subject Title : ENERGY, DIARY AND DRUG CHEMISTRY

(New Energy Sources for the New Century, Drug Chemistry)

Course Code : CHMA2EB Number of Credit Hours: 3 (Three)

Subject Description :

This course presents the Pollution-Environmental issue, New Energy Sources for the New Century, Drugs Chemistry, Dairy Chemistry and Agricultural Chemistry.

Goals:

To enable the students to learn the applications of “Chemistry what is in day- to-day life”.

Objective:

On successful completion of the course the students should have:

Understood what is present in the environment

Learnt how to solve the environmental issues

Learnt about drugs chemistry.

UNIT-1


Chemistry of global warming-green house effect-earth’s energy balance-vibrating molecules and the green house effect-molecular response to radiation-methane and other green house gases-climate modeling-Neutralizing the threat of acid rain.
UNIT-II

NEW ENERGY SOURCES FOR THE NEW CENTURY: Renewable energy sources-
Introduction to Solar energy-Waste Bio-Mass energy-Sea wave energy-Tidal energy-Ocean thermal conversion energy-Geothermal energy-Wind energy-Nuclear fusion energy.


Nuclear energy- nuclear fission and fusion-production of electricity by nuclear reactor-radioactivity and the hazards of radioactivity-living with nuclear power.

UNIT –III

DRUGS CHEMISTRY: Antibacterial Drugs-Sulpha drugs, (ii) Antibiotics-Sulphanilides-
Properties of Sulphanilamides, Mechanism of Action of Sulpha drugs, Sulphanilamide, Sulphadiazine, Cibazole, Sulphafurazole, Prontosil; Antibiotics; Classification of Antibiotics; Chloramphenical; Penicillin; Streptomycin; Tetracycline; Macrolides.

Anticonvulsant Agents-Barbiturates-Synthetic uses; Mydantoin; Oxazolinediones; Acetyl Urea derivatives; Succinimides; Miscellaneous.

Acquired Immuno Deficiency Syndrome (AIDS)-Introduction; Prevention; Treatment-
Heterocyclic compounds as (eg., Quinoline, Carbazole, Coumarin and Naphthyridines)-HIV Integrase Inhibitors – Anti-HIV natural products - Synthesis.

Awareness through chickun-guinea-Chikungunya, Causes; Virus; mosquito; Emergent in drug discovery- Comparative studies with malaria.

UNIT-IV

DAIRY CHEMISTRY: Milk and Milk products-Composition of Milk; Flavour and aroma of Milk; Physical properties of Milk; Effect of heat on Milk; pasteurization; Homogenisation; milk products; Cream; butter; ice cream; milk powder
UNIT-V

AGRICULTURAL CHEMISTRY: Soil Chemistry- Introduction; Soil classification & survey; Properties of Soil; Soil Texture; Soil Water; Soil Temperature; Soil Colloids; Soil Minerals; Soil pH acidity and alkalinity; Buffering Soil; Soil Fertility; Soil formation.

Insecticides, Fungicides and Herbicides- Introduction; Methods of Pest Controls; Methods of using Pest Controls; insecticides; the arsenic compounds; Fluorine compounds; Boron compounds; Mercury compounds; Copper compounds; Sulphur compounds; Modern Insecticides; Some Important Herbicides; Rodenticides; Benefits of Pesticides; Adverse Environmental effects of pesticides.

Fertilizers- Classification of Fertilizers; Important example for Fertilizers; Nitrogenous fertilizers, Phosphate fertilizers, Potash fertilizers; Effects of fertilizers.

Manures, compost and saw dust- Farm yard Manure; Compost; Reinforcing Manure; Green Manure Crops; Saw dust; Night soil, sewage and sludge; Bio gas production and Manure.

REFERENCES


4) Fundamental Concepts of Applied Chemistry, Jayashree Ghosh, S.Chand, 2005


CORE PRACTICALS

Subject Title: INORGANIC PRACTICALS

Course No. CHMA23P

Number of credit hours : 4(four)

Subject Description:

This practical deals about the quantitative and qualitative analyses and estimation of metal ions.

Goals:
To motivate the students to understand the basic principles of lab techniques adopted in inorganic laboratories

Objectives:

On successful completion of the course the students should have

(i). Learnt about the quantitative and qualitative analyses and colorimetry.

(ii) Learnt the estimation metals using photoelectric colorimeter.

Contents

1. Qualitative analysis:

Qualitative analysis employing semi-micro methods and spot tests of mixtures of common cations and ions of the following less familiar elements.

Molybdenum, tungsten, selenium, tellurium, cerium, thorium, titanium, zirconium, vanadium, uranium and lithium.

2. Colorimetry:

Colorimetric estimations of copper, nickel, iron and chromium using photoelectric colorimeter.

3. Industrial analysis:

(i) Analysis of two of the following alloys: brass, bronze, stainless steel, solder type metal.

(ii) Analysis of any one of the following: cement, glass, ultramarine.

(iii)
4. **Titrimetry:**

Complexometric titrations involving estimations of calcium, magnesium, nickel, zinc and hardness of water.

5. **Quantitative analysis:**

Quantitative analysis involving volumetric and gravimetric estimations of at least four mixtures of cations.

6. **Preparation of inorganic complexes:**

About six preparations involving different techniques selected from the following.

(i) Potassium tris(oxalato)aluminate  
(ii) Nickel ammonium sulphate  
(iii) Tris(thiourea)copper(I) chloride  
(iv) Potassium tris(oxalato)ferrate  
(v) Hexamminecobalt(III) chloride  
(vi) Ammonium hexachloro stannate(IV)  
(vii) Tetrammine copper(II) sulphate  
(viii) Cis and trans bis(glycinate) copper.
SUPPORTIVE - II

Subject Title: CHEMISTRY IN DAY TO DAY LIFE

Course No. GS73

Number of credit hours: 2(two)

Subject Description: This supportive paper deals with the basic chemistry in day-to-day life

Goals: To enable the student to understand about the manufacture of commercial products.

Objectives: After completion of the course the students should have understood the biological implications, industrial products and preparations etc.

Contents

Unit - I

Carbohydrates - Proteins - Lipids - Nucleic acids and Vitamins – Definition, Sources, Classification, Applications and Diseases due to deficiency.

Unit - II


Unit - III


Unit - IV

CORE VII

Subject title : ORGANIC CHEMISTRY-III
(Spectroscopy & Organic Photochemistry)

Course Code : CHMA33A Number of credit hours : 4(four)

Subject Description:

This course presents the basic principles of NMR, Mass Spectroscopy, Photochemistry and Pericyclic Reactions.

Goals:

To enable the students to learn the theories of photochemistry and Spectroscopic techniques and its applications.

Objectives:

On successful completion of the course the students should have

i) Learnt the basic principles of Mass and NMR spectroscopy and application in organic molecules

ii) Learnt the basic principles of photochemistry and electrocyclic reactions

iii) Learnt the stereochemistry involved in pericyclic reactions.

Contents

Unit – I

Mass Spectroscopy:

Presentation and analysis of spectra - determination of molecular formula - nitrogen rule - isotopic abundance analysis - metastable ions and peaks - the molecular ion peak.

Fragmentation process - symbolism (scission only) - even and odd electron ions - scission with rearrangement - Retro Diels-Alder rearrangement - McLafferty rearrangement - double band and (or) ring equivalents implied from a formula.
Fragmentation associated with functional groups - aliphatic compounds - aldehydes - ketones - carboxylic compounds - esters - amides - alcohols - thiols - amines - ethers - sulphides and halides - aromatic compounds - eliminations due to ortho group.

Unit – II

Nuclear Magnetic Resonance Spectroscopy:

Magnetic properties of nuclei - theory of nuclear resonance - chemical shifts - spin-spin coupling - shielding and deshielding mechanisms - chemical exchange - applications of NMR to organic compounds - nuclear magnetic double resonance - resonance with other nuclei - $^{13}\text{C}$ NMR (elementary idea only).

Applications of organic spectroscopy:

Structure determination of organic compounds by using UV-Vis, IR, $^1\text{H}$ & $^{13}\text{C}$-NMR and Mass spectroscopic techniques (simple molecules only – restricted to 12 carbon systems with/without one hetero atom).

Unit – III

Photochemical Excitation and Ketone Photochemistry:


Unit- IV

Photochemistry of Alkenes and Aromatic Compounds:

Olefin photochemistry – conjugated olefins – Isomerisation and rearrangements – Cis trans isomerisation – valence isomerisation – rearrangement of 1,4 and 1,5 dienes – di-pi-methane rearrangement - Cope and Claisen rearrangement – cycloaddition reactions – Photochemistry of Aromatic compounds – Arene photoisomerisation – Photodimerisation – Cycloaddition reactions – 1,2 cycloadditions – Photooxygenation – ene reaction.
Unit- V

Pericyclic Reactions and their Stereochemistry:


References

Subject title : INORGANIC CHEMISTRY-III

(Solid state chemistry and Nuclear chemistry)

Course Code: CHMA33B

Number of credit hours : 4(four)

Subject Description:

This course emphasizes the elaborate account of crystallographic data of various compounds, defects in crystal structure and also describes the nuclear chemistry in depth.

Goals:

To make the student to understand about the crystal structures and nuclear chemistry.

Objectives:

On successful completion of the course the students should have

i) thorough knowledge about the X-ray crystal structure of the compounds

ii) analytical tools which are used in nuclear chemistry

Contents

Unit - I

The growth and form of crystals - the crystal systems and Bravais lattices - Miller indices and labelling of planes - symmetry properties - crystallographic point groups and space groups - fundamentals of X-ray diffraction - powder and rotating crystal methods - systematic absences and determination of lattice types - analysis of X-ray data for cubic system - structure factor and Fourier synthesis - electron and neutron diffraction and structure determination.

Unit - II

Unit - III

Metallic state - free electron and band theories - non - stoichiometry - point defects in solids - Schottky and Frenkel defects - linear defects - dislocations - effects due to dislocations - electrical properties of solids - insulators - intrinsic semiconductors - impurity semiconductors (n and p- type) and superconductors - elementary study of liquid crystals.

Unit - IV

Nucleus: nuclear structure - stability of nuclei - packing fraction - even - odd nature of nucleons - n/p ratio - nuclear potential - binding energy and exchange forces - shell model and liquid drop model.

Decay of radionuclei: rate of decay - determination of half-life period - secular equilibrium and decay series.

Modes of decay: alpha, beta, gamma and orbital electron capture - nuclear isomerism - internal conversions - Q value - nuclear cross section - threshold energy and excitation functions.

Particle acceleration and counting techniques: linear accelerator - cyclotron and synchrotron - betatron - G. M. counter - proportional and scintillation counters.

Unit - V

Different type of nuclear reactions with natural and accelerated particles - transmutation - stripping and pick-up - spallation - fragmentation, etc. - fission - characteristics of fission reaction - product distribution and theories of fission - fissile and fertile isotopes - U235, U238, Th232 and Pu239 - atom bomb - nuclear fusion - stellar energy - synthesis of new elements - principles underlying the usage of radioisotopes in analysis - agriculture - industry and medicine - mechanism of chemical reactions - uses of radioisotopes in analytical chemistry - isotopic dilution analysis - neutron activation analysis and dating methods.

References

1. W.J.Moore – Physical Chemistry
2. L.V.Azroff – Introduction to solids
3. W.E.Addision – structural principles of Inorganic Chemistry
4. N.B.Hannay – Solid state chemistry
5. R.A.Alberty – Physical chemistry
6. S.Glasstone – Source book on atomic energy
7. G.Friedlander, J.W.Kennedy, - Nuclear and Radiochemistry
   E.S.Macias and J.M.Miller
CORE IX

Subject title: PHYSICAL CHEMISTRY – III
(Chemical Kinetics, Surface Chemistry and Macromolecules)

Course Code. CHMA33C Number of credit hours: 4(four)

Subject Description:
This course focuses on the rate and order of various reactions, theories of reactions, catalytic activity and their mechanisms and polymer chemistry.

Goals:
To make the students to understand about the chemical kinetics and effects on the rate of the reaction.

Objective:
On successful completion of the course the students should have
i) Detailed knowledge about the rates and various parameters which affects the rate.
ii) Theories of catalytic activity and polymerization techniques

Contents

Unit - I CHEMICAL KINETICS

Unit - II KINETICS OF REACTION IN SOLUTION
Comparison between gas phase and solution reactions – Cage effect – The influence of the solvent on the reactions between ions and reaction between ions and neutral molecules –
Influence of ionic strength on rates of reactions in solution – Significance of volume and entropy of activation – Secondary salt effect - Kinetic treatment of complex ion.

Parallel reactions of the same order (first or second order) – Reversible reaction of the same order (first or second order) – First order forward and second order backward – Consecutive first order reactions, steady state and rate determining step (or equilibrium) approximation of complex reactions – Chain reactions and explosions.

**Unit - III  FAST REACTIONS**

Study by stop-flow techniques, relaxation methods – Flash photolysis, magnetic resonance methods - Kinetic theory of gases and its Postulates – Maxwell distribution of Molecular velocities - Expressions for most probable velocity, average velocity, root mean square velocity – Collision diameter, Collision frequency, Mean free path. Transport properties of gases – Thermal conductivity, Viscosity, Diffusion - principle of equipartition of energy.

**Unit - IV  HOMOGENEOUS CATALYSTS**

Specific and general acid-base catalysis – Bronsted catalysis law – Acidity functions. Enzyme catalysis (single substrate reactions only) – Michaelis-Menton kinetics – Influence of pH and temperature on enzyme catalysis.


**Unit - V  MACROMOLECULES**


**References**

3. P.W. Atkins, Physical Chemistry
4. W.J. Moore, Physical Chemistry, Longmans
Subject Title : BIO-ORGANIC CHEMISTRY

(Retro synthesis, Bio-Organic, Bio-Energetics, Novel Reagents and Medicinal Chemistry)

Course Code: CHMA3EA   Number of credit Hours : 3 (Three)

Subject Description: This paper deals with organic chemistry in biology and their applications

Goal:
1. To teach the students the organic essential role in biology
2. To teach the synthetic organic methodologies.
3. To teach novel reagents involved in organic reactions
4. To teach the medicinal chemistry

Objective:
On completion of the course the students should have:
Understood role and application of organic chemistry role in biology
Clinical skills in biology by using organic knowledge
Learnt the knowledge of organic reagents in biology.

Contents

Unit I:
Retrosynthetic analysis, Protection and Deprotection

An introduction to retrosynthesis - synthon – synthetic equivalent – target molecule, functional group interconversion. Retro synthetic analysis and Synthesis of simple organic molecules such as 1,2, 1,3, 1,4 and 1,5 dicarbonyl compounds both acyclic and cyclic. Formation of 3, 4, 5 and 6 membered cyclic compounds. Use of standard reactions, like Grignard reactions, Robinson annulations. Protection and deprotection of functional groups (R-OH, RCHO, R-CO-R, R-NH₂ and R-COOH). Use of PTC (Phase-transfer catalyst) and Crown ethers in organic synthesis.
Unit II:

Bio-Organic Chemistry:

Pyrimidines (cytocine and uracil) and purines (adenine and guanine only).

Nucleic acids - structure and synthesis of nucleosides - structure and synthesis of nucleotides - Structure of RNA and DNA and their biological importance.

UNIT III:

Bio-Energetics:

Concept of energy – thermodynamic principles – first law, second law, combining the two laws – relationship between standard free energy change and equilibrium constant. Standard free energy values of chemical reactions – Adenosine triphosphate (ATP) as universal currency of free energy in biological systems – ATP hydrolysis and equilibria of coupled reactions – inter conversion of adenine nucleotides.

Unit IV:

Novel Reagents in Organic Synthesis:

Synthesis and applications of Organolithium, Organomagnesium, Organozinc and Organo Copper reagents. Modern synthetic methods: Metal mediated C-C coupling reactions: Mechanism and synthetic applications of Heck, Stille, Suznki, Negishi, Sonogashina, McMurray, Metathesis, Carbonylation reactions.

UNIT V:

Medicinal Chemistry:


Metals in Drug design: Historical development and advantages-Immunopharmacology and drug development.
References


ELECTIVE VI

Subject Title: INDUSTRIAL ORGANIC CHEMISTRY
(Industrial Organic Syntheses, Dyes, Oils, Fats, Waxes, Soaps and Polymers)

Course Code: CHMA3EB
Number of credit Hours: 3 (Three)

Subject Description: This paper deals with the industrial syntheses of petrochemicals, applications of dyes, and industrial oriented applications of oils, fats, soaps.

Goal:
1. To teach the students the essential role of petrochemicals
2. To teach methodologies involved in dyeing.
3. To teach preparation of soaps, oils and waxes
4. To teach the chemistry of natural polymers.

Objective:
On completion of the course the students should have:
Understood role and application of petrochemicals
Preparative skills in manufacturing soaps, dyes and waxes.
Learnt the knowledge of natural polymers as their behaviour.

Unit –I
Industrial Organic Syntheses-Petrochemicals:
Introduction-Raw material and basic processes-chemical processes used in industrial organic synthesis-petrochemicals-methanol-ethanol-rectified spirit from beer-methylated spirit-proof spirit-preparation of absolute ethanol from rectified spirit-acetaldehyde-acetic acid-isopropanol-ethylene glycol-glycerine-acetone-phenol-ethylacetate.

Unit –II
Hydrocarbons from Petroleum:
Aromatic hydrocarbons-benzene, toluene, xylenes-chemical processing of paraffin hydrocarbons, -acetylene and aromatic hydrocarbons.

Unit-III

Dyes:

Introduction-sensation of colour-colour and constitution-nomenclature-basic operations in dyeing-classification of dyes according to the mode of application.-synthesis, reaction and applications of diphenylmethane dyes-triphenylmethane dyes-phthalein dyes-xanthene dyes-acridine dyes-sulphur dyes-cyanine dyes.

Unit-IV

Oils, Fats, Waxes and Soaps:


Unit-V

Natural and Synthetic Polymer:

Introduction-types of polymerization and their utility, mechanism involved in preparation-thermoplastic and thermosetting polymers-phenolic resins, polurethanes, epoxyresins, alkyd resins. Natural and synthetic rubber-types and their utility-polymer properties and structure.

References:

1. *Industrial Chemistry (Including Chemical Engineering)* -- B.K.Sharma (10th Edition)
CORE PRACTICALS

Subject Title: PHYSICAL CHEMISTRY PRACTICALS

Course Code. CHMA33P Number of credit hours : 4(four)

Subject Description:
This practical deals about the experiments in chemical kinetics, conductivity and potentiometric titrations.

Goals:
To motivate the students to understand the principles of chemical kinetics, potentiometric and conductometric titrations.

Objectives:
On successful completion of the course the students should have
(i) Learnt about experiments on chemical kinetics
(ii) Learnt the potentiometric and conductometric titrations

Contents
1. Chemical kinetics (I and II order) - 5 Nos.
   (Determination of rate constant of acid catalysed hydrolysis of an ester,
   Determination of Arrhenius parameters, kinetics of persulphate - iodine reaction,
   study of primary salt effect, kinetics of iodination of acetone)

2. Molecular weight determination - 1 No.
   (Rast method)

3. Phase study - simple eutectic system - 1 No.

   (partition coefficient of I₂, the study of equilibrium of the reaction between KI and iodine)

5. Conductivity experiments - 6 Nos.
   (acid - base titration, mixture of acids vs NaOH, precipitation titrations, mixture of halides,
   Determination of dissociation constant, verification of Debye - Huckel Onsagar equation and
   Kohlraush law)

6. Potentiometry - 5 Nos
   (i) redox titrations
   (ii) acid - base titrations
   (iii) precipitation reactions

7. Validation of Freundlich adsorption isotherm.

8. Determination of unknown concentration of the given solution using photoelectric colorimeter.
SUPPORTIVE III

Subject Title: CHEMISTRY OF ENVIRONMENT

Course Code. GS Number of credit hours: 2(two)

Subject Description: This supportive paper deals with the applied chemistry in environment.

Goals: To enable the student to understand about the commercial products.

Objectives: After completion of the course the students should have understood the soil effects, essential inorganic compounds, role of milk, industrial preparations of oil, fat etc.

Contents

Unit – I

Soil-Introduction-Definition-Classification of Soil- Environmental properties of Soil-Soil minerals-Soil contamination- Ecological and health effects of Soil contamination.

Unit – II

Medicinal inorganic compounds-Alum, Phosphoric acid, Ferric ammonium citrate: Preparation, Properties and uses. Biological role of inorganic compounds-Sodium, Potassium, Calcium and Iodine: Sources, biological role and deficiency.

Unit – III


Unit - IV

Subject Title: ORGANIC CHEMISTRY – IV
(Aromaticity, Green Chemistry, Alkaloids, Steroids and Organic Synthesis)

Course Code: CHMA43A  Number of credit hours: 4 (four)

Subject Description:
This course gives the knowledge about the basics of organic chemistry, which involves aromaticity, chemistry of alkaloids and steroids and route to organic synthesis with the help of novel reagents.

Goals:
To make the students understand about the concept of aromaticity and factors affecting the same. Various novel chemical reactions which are used for organic synthesis are also well explained

Objectives:
On successful completion of the course the students should have
1. a versatile knowledge of aromaticity, different naming reactions and their application in organic synthesis
2. learnt the identification of molecular structures

Contents

Unit - I

Aromaticity:

Green Chemistry:
Designing a green synthesis, basic principles of green chemistry- Elementary idea of Microwave and Sono chemistry

Unit – II

Alkaloids:
Unit - III

Steroids:


Unit – IV

Named reactions:

Baylis-Hillman reaction, Mannich, Simmons – Smith, Reformatsky, Ullmann, Wittig–Horner, Peterson, Acyloin condensation, Robinson annihilations, Oppenauer oxidation, m-CIC₆H₄COOOH.

Functional group transformations:

Carbonyls (aldehyde and ketone)- Preparation from alcohols, alkenes, alkynes, arenes and carboxlic acid derivatives. Reactions: Nucleophilic additions-cyanide, bisulfate, ammonia, amines, oximes, hydrazines, semicarbazide, hydride, hydrogen, organometallic reagents, Cannizaro and Benzoin condensation reactions. Reaction of enones-1,2- and 1,4-additions. Oxidation of carbonyl compounds and Wittig reaction.

Amines (both aliphatic and aromatic)-Methods of preparation of amines by reduction of nitro compounds, imine, amides and cyanides, Hofmann degradation of amides and ammonolysis of halides.Reactions-basicity and acidity of different amines, salt formation, alkylation, acylation, Hofmann elimination and diazonium formation and its reactions. Reactions of aromatic amines

Unit – V

Reagents in Organic Synthesis:

Use of the following reagents in Organic synthesis and functional group transformation.

Diborane, LiAlH₄, Ozone, OsO₄, DCC, 1,3-Dithiane, LTA, Peracetic acid, Raney Nickel, PPA, CH₃N₂, Tri-n-butyl tin hydride, n-Butyl lithium, NBS, DDQ, DBU (Diaza bicyclo-undecane), SeO₂, Tri methyl silyl iodide, Gilman’s reagent, Lithium dipropyl amide.
References

1. L.G.Wade Jr., Organic chemistry.
Subject Title: INORGANIC CHEMISTRY – IV  
(Organometallic chemistry)

Course Code: CHMA43B Number of credit hours: 4(four)

Subject Description:
This course presents the detailed study of synthetic organometallic complexes and their applications towards homo and heterogeneous catalysis.

Goals:
To make the students to understand different reactions leading to the formation of various organometallic complexes and the mechanism involved.

Objectives:
On successful completion of the course the students should have
1. Learnt the detailed study of synthetic organometallic complexes owing to the preparation as well as their reactivity and application which is very useful in the modern era.

Contents

Unit - I

Unit - II
Unit - III

Unit - IV

Unit - V

References
CORE XII

Subject Title: PHYSICAL CHEMISTRY – IV
(Classical and Statistical thermodynamics)

Course Code. CHMA43C Number of credit hours: 4(four)

Subject Description:
This paper describes laws of thermodynamics and various co-efficient involved in thermodynamics with respect to their applications.

Goals:
To develop a vast knowledge in the interpretation of various physical quantities involved in thermodynamics.

Objectives:
On successful completion of the course the students should have learnt about the fundamentals of classical and statistical thermodynamics and their applications.

Contents

Unit – I THERMODYNAMICS AND NON-IDEAL SYSTEMS

Chemical potential and the definition of fugacity – Determination of fugacity of gases by graphical method and from equations of state – Variation of fugacity with temperature – Fugacity and the standard state for non-ideal gases – Fugacity (or activity) coefficient – Fugacity and mixtures of non-ideal gases, chemical equilibrium involving non-ideal gases.


Unit – II THIRD LAW OF THERMODYNAMICS

Probability and third law – Need for the third law – Nernst heat theorem and other forms stating third law – Thermodynamic quantities at absolute zero – Statistical meaning of third law and apparent exception.

Mathematical introduction

**Unit – III: STATISTICAL THERMODYNAMICS - I**


**Unit – IV: STATISTICAL THERMODYNAMICS - II**


**Unit – V: STATISTICAL THERMODYNAMICS - III**

**Bose-Einstein and Fermi-Dirac Statistics:**


**Heat capacities of Solids:**

Einstein’s and Debye’s theories of heat capacities of solids.

**References:**

CORE XIII

Subject Title: ANALYTICAL CHEMISTRY

Course Code. CHMA 43D

Number of credit hours : 4(four)

Subject Description:

This course presents the basic principles of quantitative inorganic analysis and related topic and chromatographic methods.

Goals:
To motivate the students to understand the basic principles of analytical chemistry

Objectives:

On successful completion of the course the students should have

i) Learnt about the various methods involved in analytical techniques

ii) Expertise in chromatography of various types

Contents

Unit I : Quantitative Inorganic Analysis

Theoretical basis of quantitative inorganic analysis-common ion effect solubility product, effect of acid, temperature and solvent upon the solubility of a precipitate. Super saturation-Von Weimarn concept. Formation and treatment of precipitates-co precipitation and post-precipitation. Precipitation from homogeneous solution. Specific and selective precipitants.

Principles of acid-base, oxidation-reduction, precipitation and complexometric titrations-indicators used in such titrations. Uses of organic reagents in inorganic quantitative and qualitative analysis.

Unit-II : Data Analysis

Unit-III : Techniques in Inorganic Chemistry


Unit-IV : Electrochemical Methods of Analysis

Cyclic Voltammetry, coulometry and amperometry-principle and applications. Thermal Characterization techniques, Principle and applications of Differential Thermal Analysis (DTA), Differentials Scanning Calorimetry (DSC) and Thermogravimetric Analysis (TGA) Thermometric titration.

Unit- V : Chromatographic methods

Classification – techniques and applications in column, size-exclusion, ion exchange, paper and thin layer chromatography. Gas chromatography and high performance liquid chromatography (HPLC) – principle, equipment design, sample injection system, columns, detectors and applications.

References:

2. G.D. Christian – Analytical Chemistry
4. D.A. Skoog – Instrumental Methods of Analysis.