

BHARATHIAR UNIVERSITY: COIMBATORE – 641 046.
M.Sc. Chemistry (Univ. Dept.) – 2014-2015 onwards
Under choice based credit system (CBCS)

S No.	Paper Code	General Title	Specific Title of the paper	Credit/Marks
Semester I				
1.	CHMA13A	Organic Chemistry-I	Reaction mechanisms	4/100
2.	CHMA13B	Inorganic Chemistry-I	Coordination Chemistry	4/100
3.	CHMA13C	Industrial Chemistry-I	Applied Bio-Inorganic Chemistry	4/100
4.	CHMA1EA	Elective – I	Analytical Chemistry	4/100
5.	CHMA13P	Practicals-I	Organic Practicals	4/100
6.	1GS	Supportive-I	Offered from other Departments	2/50
Semester II				
7.	CHMA23A	Organic Chemistry –II	Natural Products, Proteins, Nucleic Acids, Stereochemistry	4/100
8.	CHMA23B	Physical Chemistry-I	Quantum Chemistry and Electrochemistry	4/100
9.	CHMA23C	Industrial Chemistry-II	Water treatment, fuels and Polymers	4/100
10.	CHMA2EB	Elective-II	Physical Methods in Chemistry.	4/100
11.	CHMA23P	Practicals-II	Inorganic Practicals	4/100
12.	2GS	Supportive-II	Offered from other Departments	2/50
Semester III				
13.	CHMA33A	Inorganic Chemistry-II	Solid State Chemistry and Nuclear Chemistry.	4/100
14.	CHMA33B	Physical Chemistry-II	Kinetics, Surface Chemistry, Macro molecules and kinetic theory of gases.	4/100
15.	CHMA33C	Industrial Chemistry-III	Industrial Organic Syntheses, Dyes, Oils, Fats, Waxes & Soaps, Polymers	4/100
16.	CHMA3EC	Elective-III	Organic Photo Chemistry	4/100
17.	CHMA33P	Practicals –III	Physical Chemistry Practicals	4/100
18.	3GS	Supportive-III	Offered from other Departments	2/50
Semester IV				
19.	CHMA43A	Organic Chemistry-III	Aromaticity, Alkaloids, Steroids and Organic Synthesis	4/100
20.	CHMA43B	Inorganic Chemistry-III	Organometallic Chemistry	4/100
21.	CHMA43C	Physical Chemistry-III	Classical and Statistical Thermodynamics	4/100
22.	CHMA43D	Industrial Chemistry-IV	New Energy Sources for the New Century, Drug Chemistry	4/100
23.	CHMA4LV	Project work	--	8/200
Total				90/2250

As per the CBCS, each PG student is allowed to choose 3 supportive courses offered by the other departments of the university.

Supportive Courses for Other Department Students:

1. Applying Chemistry to Society; 2. Chemistry in Day to Day Life

CORE I

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 outline the mechanism and discuss the application 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 electrophilic, 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.

SN_1 , SN_2 , SN_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:

SE_1 and SE_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 Bischoff-Napieralski reaction) - haloalkylation - aminoalkylation and amidoalkylation - thioalkylation -acylation with nitriles (Hoesch reaction) - cyanation - hydroxylation.

Unit - III

Molecular Rearrangements:

Molecular rearrangements - intramolecular rearrangements - 1,2- shifts in carbonium ions - Wagner-Meerwein and related rearrangements - Demjanov rearrangement - migration to carbonyl carbon - Neber rearrangement -Benzilic acid- Baeyer-Villiger rearrangement -

rearrangements to electron deficient nitrogen and oxygen - dienone-phenone - Favorski - Wolf - benzidine - Claisen - Cope rearrangement, Ylides:Stevens-Wittig-Sommelet-Gruvenstein-Zimmermann rearrangements- non-cyclic rearrangements - Chapman - Wallach rearrangement.

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.

Mannich reaction - Meerwein-Ponndorf reduction - Grignard reactions - Aldol - Claisen - Stobbe - Darsen - Wittig - Thorpe and benzoin condensations - Cannizarro reaction. Elimination reactions - E1 and E2 mechanisms - orientations - Hofmann and Saytzeff rules - elimination versus substitution - Chaugav reaction - Hofmann degradation and Cope elimination - dehydration of alcohols - dehydrohalogenation - mechanisms and orientation in pyrolytic elimination.

Unit - V

Oxidation and Reduction:

Formation of C=C, C-C bonds by dehydrogenation - dehydrogenation by quinones, SeO_2 , $\text{Hg}(\text{OAc})_2$, and $\text{Pb}(\text{OAc})_2$ - 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 - catinanes.

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

References

1. Jerry March, Advanced organic chemistry - Reactions, mechanism and structure, Mc Graw Hill Kogakusha Ltd., 1977.
2. Lowry and Richardson, Mechanism and theory in organic chemistry, Harper & Row Publishers, New York 1981.
3. Mukergee and S. P. Singh, Reactions mechanisms in organic chemistry, Mc Millan 1976.
4. Raj K.Bansal Organic Chemistry Reaction mechanisms, Mc.Graw-Hill Publishing Company Ltd, 2006

CORE II

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 structure 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 spinals - 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 fields 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 - optical isomerism in octahedral complexes - absolute configuration of complexes - stereoselectivity and conformation of chelate rings - coordination number seven and eight.

Unit - V

Inorganic chains - rings - cages and clusters - catenation - heterocatenation - intercalation chemistry - one dimensional conductor - isopolyanions - heteropolyanions - borazines - phosphazenes - phosphazene polymers - ring compounds of sulphur and nitrogen - homocyclic inorganic systems - cages - boron cage compounds - metal clusters - dinuclear clusters - trinuclear clusters - tetranuclear clusters - hexanuclear clusters - structural prediction of organometallic clusters.

References

1. Inorganic Chemistry - Principles of structure and reactivity, Fourth Edition
J. E. Huheey, E. A. Keiter and R. L. Keiter - Addison Wesley Publishing
Co, NY, 1993.
2. Advanced Inorganic Chemistry - F. A. Cotton and G. Wilkinson
3. Mechanism of Inorganic reactions - F. Basolo and R. G. Pearson
4. Inorganic Chemistry - R. B. Heslop and P. L. Robinson
5. Introduction to Ligand Fields - B. N. Figgis - Wiley Eastern Ltd, New Delhi, 1976.

CORE III

**Subject Title: INDUSTRIAL CHEMISTRY- I
(APPLIED BIO-INORGANIC CHEMISTRY)**

(Applied Bioinorganic Chemistry , Principles, Inorganic drug targets and Metals in medicine)
Course Code : CHMA13C Number of Credits :3 (Three)

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 – Phorphyrin system – Structure and functions of Hemoglobin and Myoglobin – Dioxygen binding, transport and utilization - Structure and functions of Chlorophyll.

Unit - II

Metalloenzymes – Definition – Examples - Structure and functions of — Carboxy peptidase-A and Carbonic anhydrase – Superoxide dismutase (SOD) — Xanthine oxidase - Nitrogenase – Vitamin B12 co-enzyme – Non-Heme iron-sulphur proteins - Ferridoxins – Rubredoxins – Cytochrome C - Blue copper proteins – Plastocyanin.

Unit - III

Applications of physical methods to bioinorganic chemistry (Exclusive of Instrumentation) – X-ray absorption spectroscopy (XAS) and Extended X-ray absorption fine structure (EXAFS) – Nuclear magnetic resonance spectroscopy (NMR) and Electron paramagnetic resonance method (EPR) – Mossbauer spectroscopy – Circular dichroism (CD) - Electronic spectroscopy (UV-visible and fluorescence emission)

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.

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 - Cancer chemotherapy- Bioinorganic chemistry of platinum and ruthenium anticancer drugs - Mechanism of action of *cis*-platin - Clinical trials and their significance - Applications of Coordination complexes in medicine and agriculture

References:

1. I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine ,Bioinorganic Chemistry; University Science Books .
2. Dr Asim R Dass, Bioinorganic Chemistry 2007. Books and Allied (P) Limited. Lawrence Que,Jr , Physical Methods in Bioinorganic Chemsity.
3. Lawrence Que, Jr, Physical Methods in Bioinorganic Chemistry – Spectroscopy and Magnetism.
4. J.E.Huheey, E.A.Kieter Inorganic Chemistry 4th Edition,
5. R.L.Keiter Addison Wesley Publishing Company.

ELECTIVE-I

Subject Title: ANALYTICAL CHEMISTRY

Course No. CHMA 1EA

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

Errors in chemical analysis – Defining terms: mean, median, accuracy and precision – classification of errors: Systematic errors and random errors. Improving accuracy of analysis – mean, standard deviation and Q-test. Comparison of results – Least square, ‘t’-test, ‘F’-test and ‘Chi’ square test.

Unit-III : Techniques in Inorganic Chemistry

Colorimetry: Theoretical and practical aspects of colorimetric analysis. Flame emission and atomic absorption spectroscopy – types of atomic spectroscopy – emission methods – absorption methods – fluorescence methods – source and atomizers for atomic spectroscopy – flame atomizers – Electrothermal atomizers – principle and applications of atomic absorption spectroscopy. Advantages of atomic absorption spectrometry over flame photometry.

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), Differential 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:

1. A.T. Vogel – A text book of Quantitative Inorganic Analysis.
2. G.D. Christian – Analytical Chemistry
3. D.A.Skoog and D.M.West – Fundamentals of Analytical Chemistry.
4. D.A. Skoog – Instrumental Methods of Analysis.
5. Skoog, West, Holler and Crouch – Analytical Chemistry – An Introduction.

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 by named reaction

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-Bromoacetanilide from acetanilide
- (vi) m-Dinitro benzene from nitrobenzene
- (vii) Picric acid from phenol
- (viii) 2-Naphthylbenzoate from 2-naphthol.

CORE IV

**Subject Title: ORGANIC CHEMISTRY-II
(NATURAL PRODUCTS, PROTEINS, NUCLEIC ACIDS, STEREOCHEMISTRY)**

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, synthesis, bio-synthesis and elucidation of various natural products
- ii) 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, proteins and nucleic acids:

Synthesis of amino acids and polypeptides - primary and secondary structure of a protein - the N-terminal and C-terminal residue analysis - oxytocin - enzymes and coenzymes - biosynthesis of protein - nucleic acids - structure and synthesis of nucleosides - structure and synthesis of nucleotides - structure of RNA and DNA and their biological importance.

Unit - III

Conformational analysis and stereochemistry:

Geometrical and optical isomers : R, S, E, Z configurational notations - different types of optical isomerism including dissymmetric over crowded molecules - stereochemistry of sulphur and nitrogen compounds - configurations - geometrical isomerism and configurations in mono and bicyclic ring systems - conformational analysis of acyclic system - cyclohexanes - perhydrophenanthrene - decalins - carbohydrates - spiranes - allenes and biphenyls. Asymmetric Synthesis-Introduction-methods of asymmetric synthesis-auxillary controlled methods-reagent controlled methods-catalyst controlled methods.

Unit - IV

Vitamins:

Structure and synthesis of vitamin B complex : vitamin B₁ (aneurin) - vitamin B₂ (riboflavin) - pantothenic acid - folic acid - vitamin H (biotin) - vitamin B₆ (pyridoxine) - vitamin

B₁₂ (cyanocobalamin) structure only - vitamin E (α - tocopherol) - vitamin K₁ (phylloquinone) and vitamin K₂.

Unit - V

Heterocyclic compounds:

Structure - synthesis and reactions of the following systems - indole - quinoline - isoquinoline - carbazole - chromone - flavanones - flavones - flavonols - isoflavones - anthocyanins - purines - uric acid - penicillins and sulpha drugs.

References

1. I. L. Finar, Organic chemistry, vol. I and vol. II.
2. Nakanishi et. al., Natural product chemistry, vol. I, Academic press, 1974.
3. New Mann, Terpenes and Terpenoids.
5. E. L. Eliel, Stereochemistry of carbon compounds, Mc Graw Hill, 1962.
6. Acheson, Introduction to heterocyclic compounds.
7. P.Ramesh, Basic principles of Organic Stereochemistry, Meenu publication, 2005.

CORE V

Subject title : PHYSICAL CHEMISTRY – I
(QUANTUM CHEMISTRY AND ELECTROCHEMISTRY)

Course Code : CHMA23B

Number of credit hours : 4(four)

Subject Description:

This course presents the Basic principles of quantum treatment of molecules and electrochemistry

Goals:

To enable the student to learn the theories of quantum mechanical treatment, basics of electrochemistry and various applications of electrochemical phenomena

Objectives:

On successful completion of the course the students should have

- i) Learnt the knowledge of quantum chemistry and electrochemistry

Contents

Unit - I

Quantum chemistry:

Failure of classical mechanics and the success of quantum theory in explaining black body radiation - heat capacities of solids - 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

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

Solving of Schrodinger equation for the one dimensional harmonic oscillator - harmonic oscillator model of a diatomic molecule - illustration of the uncertainty principle and correspondence principle with reference to harmonic oscillator.

Unit - III

Solving of Schrodinger equation for a rigid rotor - rigid rotor model 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

Electron spin and the Pauli principles - antisymmetric nature of the wave functions - Slater determinants - approximate wave function of many electron atoms.

Need for approximation methods - the perturbation theory (first order only) application of the perturbation method of systems such as the anharmonic oscillator and He- atom - the variation method - applications of variation method to systems such as anharmonic oscillator and He-atom.

Unit - IV

Electrochemistry - Ions in solutions:

Conductivity of solutions and their measurement - the Arrhenius ionisation theory - transport numbers and mobilities of ions - measurement of transport numbers - Hittorff method and moving boundary method - ionic activities and activity coefficients and their determination by various methods - Debye-Huckel-Onsager theory - ionic atmosphere - Debye-Huckel limiting law - acids and bases - dissociation constant of acids and bases.

Unit - V

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 P^H , concentration cells with transference - electrolysis - decomposition voltages - concentration polarisation and over voltage - the polarograph.

References

1. I. N. Levine - Quantum chemistry, Prentice Hall of India Pvt Ltd, 1994.
2. R. K. Prasad - Quantum chemistry, Wiley Eastern Ltd, (1992).
3. W. J. Moore - Physical chemistry, (1962).
4. W. Castellan - Physical chemistry, (1971).
5. A. K. Chandra - Introductory quantum chemistry.
6. P. W. Atkins - Physical chemistry.
7. S. Glasstone - Electrochemistry.
8. Gordon M. Barrow - Physical Chemistry, Mc Graw Hill Publishing Company Ltd, 2007.

CORE VI

Subject Title : Industrial Chemistry-II (WATER TREATMENT, FUELS AND POLYMERS)

Course Number : CHMA23C **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

Introduction – definition, calorific value, determination of calorific value- Classification of fuels – solid, liquid and gaseous fuels, Fossil fuels, Rocket fuels and nuclear fuels - advantages and disadvantages of solid fuels over liquid and gaseous fuels. Energy – unit of energy, sources of energy, renewable and non-renewable, conventional and non-conventional energies. Solar energy – solar photovoltaic cells and applications. Energy storage: Batteries and fuel cells – dry cell (primary cell), lead –acid battery (secondary cell), hydrogen-oxygen fuel cell, advantages of fuel cell. Future options for energy – Bio conversion & advantages

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)
2. *Outlines of Chemical Technology* – For the 21st Century – M.Gopala Rao & Marshall Sittig (3rd Edition, 1997)

ELECTIVE-II

Subject Title: PHYSICAL METHODS IN CHEMISTRY
(Group theory and molecular spectroscopy)

Course No. CHMA2EB

Number of credit hours : 4(four)

Subject Description:

This course presents the basic principles of group theory and molecular spectroscopy

Goals:

To motivate the students to understand the basic principles group theory and molecular spectroscopy

Objectives:

On successful completion of the course the students should have

- (i) Learnt about the various principles involved in group theory
- (ii) learnt the principles involved in molecular spectroscopy.

Contents

Unit - I

Group theory - symmetry elements and symmetry operations - identity - centre of symmetry - axis of symmetry - plane of symmetry and improper rotation axis of symmetry.

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 - orthogonality theorem (proof not needed) and its consequences.

Construction of character table for C_{2v} and C_{3v} point groups.

Unit - II

Molecular spectra:

Ultraviolet and visible spectroscopy:

Electronic excitation - origin of different bands - intensity of bands - selection rules - laws of photometry - correlation of electronic structure with molecular structure - single chromophoric groups - conjugated systems - systems of extended conjugation and aromatic systems - instrumentation (basic idea only).

Infrared spectroscopy:

Molecular vibrations - force constant - selection rules - applications to organic and inorganic compounds - identification of functional groups - finger print region - instrumentation (basic idea only).

Unit - III

Nuclear magnetic resonance:

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}C NMR (elementary idea only).

Unit - IV

Electron spin resonance:

Theory - derivative curves - 'g' values - hyperfine splitting - isotropic and anisotropic systems - identification of free radicals - applications.

Mossbauer spectroscopy:

Isomer shifts - quadrupole interactions - magnetic interaction - mossbauer emission spectroscopy - applications.

Unit - V

Mass spectrometry:

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.

References

1. F. A. Cotton - Chemical applications of group theory.
2. Chang - Basic principles of spectroscopy.
3. R. M. Silverstein and G. C. Baseler - Spectroscopic identification of organic compounds.
4. B. P. Straughan and S. Walker - Spectroscopy (vol. I).
5. N. Banwell - Molecular spectroscopy.
6. Donald L. Pavia, Gary M. Lampman, and George S. Kriz, Jr - Introduction to Spectroscopy : A Guide for students of organic chemistry.
7. William Kemp - Organic spectroscopy.
8. D.H.Williams-Ian Fleming, Spectroscopic Methods in Organic Chemistry, Mc Graw Hill Publishing Company Ltd, 2006.

PRACTICALS II

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. Quantitative analysis:

Quantitative 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.

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.

CORE VII

**Subject title : INORGANIC CHEMISTRY-II
(SOLID STATE CHEMISTRY AND NUCLEAR CHEMISTRY)**

Course: Number CHMA33A 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

Types of solids - close packing of atoms and ions - bcc, fcc and hcp voids - Goldschmidt radius ratio - derivation - its influence on structures - structures of rock salt - cesium chloride - wurtzite - zinc blende - rutile - fluoroite - antiferite - diamond and graphite - spinel - normal and inverse spinels and perovskite - lattice energy of ionic crystals - Madelung constant - Born-Haber cycle and its applications.

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.Addison – 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
8. H.J.Arnikaar – Essentials of Nuclear chemistry.

CORE VIII

**Subject title : PHYSICAL CHEMISTRY –II
(KINETICS, SURFACE CHEMISTRY, MACRO MOLECULES
AND KINETIC THEORY OF GASES)**

Course Code : CHMA33B Number of credit hours : 4(four)

Subject Description:

This course focus 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 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

Rates of chemical reaction, kinetics of first, second and third order reactions, complex methods of determining rate laws, order and molecularity concepts.

Theories of reaction rates

Arrhenius theory, hard-sphere collision theory of gas phase reactions. Potential energy surfaces. Activated complex theory for ideal gas reactions (formation in terms of partition functions). Relation between activated complex theory and hard-sphere collision theory. Thermodynamic formulation-activated complex theory (Enthalpies and entropies of activation). Kinetic isotopic effect.

Unit-II 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, parallel first and second order reactions). 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 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.

Surface Phenomenon and Heterogeneous catalysts

Adsorption and free energy relation at interfaces. Gibb's adsorption isotherm. Physisorption and chemisorption. Adsorption isotherms (Langmuir and BET). Measurement of surface area. Kinetics of heterogeneous catalysis (Langmuir Hinshelwood mechanism and Eley-Rideal mechanism). Semiconductor catalysis.

Unit-IV Macromolecules

Addition and condensation polymers, number average and weight average molecular weights of macromolecules. Determination of molecular weights. Kinetics of polymerization, molecular and free radical mechanism. Polymerisation in solution. Stereochemistry.

Unit-V Fast reactions

Study by stop-flow techniques, relaxation methods. Flash photolysis, magnetic resonance methods.

Kinetic theory of gases

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.

References

1. K.J. Laidler, Chemical Kinetics, Tata McGraw Hill
2. Gurdeep Raj, Chemical Kinetics, Goel Publishing House.
3. P.W. Atkins, Physical Chemistry
4. W.J. Moore, Physical Chemistry, Longmans
5. A.A. Frost and R.G. Pearson, Kinetics and Mechanism, Wiley Eastern, Pvt. Ltd.
6. F.W. Billmeyer, Text book of Polymer science, Wiley- Interscience.

CORE IX

**Subject Title : INDUSTRIAL CHEMISTRY III
(INDUSTRIAL ORGANIC SYNTHESSES, DYES, OILS, FATS, WAXES & SOAPS, POLYMERS)**

Course Code : CHMA33C 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 know preparation of soaps,oils,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 and its 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-proff spirit-preparation of absolute ethanol from rectified spirit-acetaldehyde-acetic acid-isopropanol-ethylene glycol-glycerine-acetone-phenol-ethylacetate.

Unit –II

Hydrocarbons from petroleum

Introduction-raw materials-saturated hydrocarbons from natural gas-uses of saturated hydrocarbons-unsaturated hydrocarbons-acetylene,ethylene,propylene,butylenes.

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.

Introduction-Distinction between oils and fats-properties and its classifications-animal fats and oils-difference between,animal,vegetable and mineral oils-isolation of essential oils and their uses-saponification value-ester value-acid value-iodide value-wijs method-Reichert meissel value-Henher value-elaiden test-hydrogenation of oils –Soap and its manufacture-general

consideration in soap making –manufacture of toilet and transparent soaps-oil to be used for soap-cleansing action of soap.

Unit –V

Natural and Synthetic polymer.

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

Books recommended

1. *Industrial Chemistry* (Including Chemical Engineering) -- B.K.Sharma (10th Edition)
2. *Outlines of Chemical Technology* – For the 21st Century – M.Gopala Rao & Marshall Sittig (3rd Edition)

ELECTIVE-III

Subject title : ORGANIC PHOTO CHEMISTRY

Course Code : CHMA3EC

Number of credit hours : 4(four)

Subject Description:

This course presents the basic principles of photochemistry and pericyclic reactions

Goals:

To enable the student to learn the theories of photochemistry and Woodward –Hofmann rule .

Objectives:

On successful completion of the course the students should have

- i) Learnt the basic principles of photochemistry and electrocyclic reactions
- ii) Learnt the stereochemistry involved in pericyclic reactions.

Contents

Unit – I Laws of Photochemistry and Photoprimary processes

Interaction of Electromagnetic radiation with Matter-Types of excitations – Laws of Photochemistry – Grothus and Draper law – Lambert and Beer's law – Einstein law – Quantum yield – Photo primary processes ,fate of the Excited molecule – State energy diagrams – Fluorescence – Fluorescence life times – phosphorescence life times – Quenching – Stern – Volmer equation – Inter molecular processes – Photosensitisation – Predissociation – Fluorescence and structure – Triplet state and phosphorescence emission.

Unit – II Actinometry and some industrial aspects of Photochemistry

Actinometry – Light sources and their standardisation – Chemical Actinometry – Chemical reactions and their quantum yields – Gas phase photolysis – Mechanism of some typical photochemical reactions – Hydrogen Iodine – Hydrogen Bromine – Hydrogen Chlorine reactions – Photolysis of Acetaldehyde – Chemiluminescence – Mechanism – Biochemiluminescence – Photochromism – Photostabilisation – Optical brightness.

Unit – III Photochemical excitation and ketone photochemistry

Light absorption – Experimental techniques – Electronic transitions – Frank – Codon principle – Jablonski diagrams – Intersystem crossing – Energy transfer – Molecular orbital view of excitation – The Geometry of excited states – Reactivity of

Electronically excited ketones – α -cleavage - γ - hydrogen transfer Norrish Type I, Type II, Type III reactions – Photoreduction – Oxetate formation – Reactivity of π , π^* excited ketones – Photochemistry of α , β - unsaturated ketones – Optical pumping – Dienone phenol rearrangement.

Unit- IV Photochemistry of alkenes and aromatic compound

Olefin photochemistry – conjugated olefins – Isomerisation and rearrangements – Cis trans isomerisation – valence isomerisation – rearrangement of 1,4 and 1,5 dienes – di π -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

The stereochemistry of electrocyclic reactions – Symmetry properties of molecular orbitals – Symmetry control of electrocyclic reactions – perturbation theory in pericyclic reactions – Woodward Hoffmann rules – orbital correlation diagrams – The Frontier orbital theory – Electrocyclic conversion of 1,3 – dienes and 1,3,5 – trienes.

Sigmatropic reaction – Stereochemistry of sigmatropic reactions – cycloaddition – classification of cycloaddition reaction – orbital symmetry and cycloaddition – concerted Vs Non-concerted cycloaddition - 2+2 and Diel's Alder reaction – Reactivity of dienophile and diene components – orientation – stereochemistry of Diel's Alder reaction.

References

1. Fundamentals of Photochemistry – K.K.Rohatgi – Mukherjee (Revised Edition) New age International publications, Reprint 2002.
2. Physical Chemistry – Robert A.Alberty (Sixth edition) – Wiley Eastern Limited Reprint 1987.
3. Photochemistry in Organic Synthesis – edited by J.D. Coyle – Royal society of Chemistry 1986.
4. Photochemistry of heterocyclic compounds – Ole Buchardt – Wiley Interscience 1976.
5. Molecular Photochemistry N.J.Turro and W.A. Benjamin.
6. Molecular reactions and Photochemistry - Charles H.Depuy, Orville.S. Chapman, Prentice – Hall of India Pvt., Ltd. 1988.
7. Frontier orbitals and organic chemical reactions - Ian Fleming John Wiley and sons, 1976.

PRACTICALS III

Subject Title: PHYSICAL CHEMISTRY PRACTICALS

Course No. 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 the chemical kinetic experiments
- (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.**
- 4. Distribution coefficient - 2 Nos.**
(partition coefficient of I_2 , 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. Find out the validity of Freundlich adsorption isotherm.**
- 8. Determination of unknown concentration of the given solution using photoelectric colorimeter.**

Simon – Smith, Vilsmeier – Haack, Reformatsky, Ullmann, Storck Enamine, Shapiro, Wittig – Horner, Peterson, Heck Stille, Mc.Murray reaction, Ring formation by Dieckmann, Thorpe, Acyloin condensation, Robinson annulation Simmons-Smith reaction, Reduction and oxidation in synthesis, Catalytic hydrogenation, Reductions like, Wolff-kishner, Huang-Minlon modification, Birch reduction, Wolff-Kishner, Clemmensen reduction, MPV reduction, Oppenauer oxidation, $m\text{-ClC}_6\text{H}_4\text{COOH}$ reactions, Sommelet-Hauser, Wolf, Neber, Dakin, Stevens, Favorski Rearrangements.

Unit – V

Reagents in Organic Synthesis:

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

Diborane, LiAlH_4 , Ozone, OsO_4 , DCC, 1,3-Dithiane, LTA, Peracetic acid, Raney Nickel, PPA, CH_2N_2 , Tri-*n*-butyl tin hydrate, *n*-Butyl lithium, NBS, DDQ, DBU (Diaza bicyclo-undecane), SeO_2 , Tri methyl Silyl iodide, Gilman's reagent, Lithium Dimethyl cuprate, Lithium dipropyl amide.

References

1. L.G.Wade Jr., Organic chemistry.
2. I.L.Finar, Organic Chemistry, Vol.I and Vol.II.
3. L.F.Fieser and M.Fieser, Steroids, Reinbold, 1959.
4. P.J.Garrat, Aromaticity, Mc Graw Hill, 1971.
5. Jerry March Advanced Organic Chemistry.
6. Fieser & Fieser – Reagents in Organic Synthesis.

CORE XI

Subject Title: INORGANIC CHEMISTRY – III (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 leads 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

Definition of organometallic compound - 18 electron rule - effective atomic number rule - classification of organometallic compounds - the metal carbon bond types - ionic bond – sigma covalent bond - electron deficient bond - delocalised bond - dative bond - metal carbonyl complexes - synthesis - structure and reactions of metal carbonyls - the nature of M- CO bonding- binding mode of CO and IR spectra of metal carbonyls - metal carbonyls- metal carbonyl anions - metal carbonyl hydrides - metal carbonyl halides - metal carbonyl clusters -

Wades rule and isolobal relationship - metal nitrosyls - dinitrogen complexes - dioxygen complexes.

Unit - II

Metal alkyl complexes - stability and structure - synthesis by alkylation of metal halides - by oxidative addition - by nucleophilic attack on coordinated ligands - metal alkyl and 18 electron rule - reactivity of metal alkyls - M-C bond cleavage reactions - insertion of CO to M-C bonds - double carbonylation - insertions of alkenes and alkynes - insertions of metals with C-H bonds - alkylidene and alkylidyne complexes - synthesis of alkylidene complexes in low oxidation states and in high oxidation states - bonding in alkylidene complexes - synthesis and bonding in alkylidyne complexes - reactivity of alkylidene and alkylidyne complexes.

Unit - III

Alkene complexes - synthesis of alkene complexes by ligand substitution - by reduction and by metal atom synthesis - bonding of alkenes to transition metals - bonding in diene complexes - reactivity of alkene complexes - ligand substitution - reactions with nucleophiles - olefin hydrogenation - hydrosilation - Wacker process - C-H activation of alkenes - alkyne complexes - bonding in alkyne complexes - reactivity of alkynes - alkyne complexes in synthesis - cobalt catalysed alkyne cycloaddition.

Unit - IV

Cyclopentadienyl complexes - metallocenes - synthesis of metallocenes - bonding in metallocenes - reactions of metallocenes - $\text{Cp}_2\text{Fe}/\text{Cp}_2\text{Fe}^+$ couples in biosensors - bent sandwich complexes - bonding in bent sandwich complexes - metallocene halides and hydrides - metallocene and stereospecific polymerisation of 1-alkenes - cyclopentadiene as a non-spectator ligand - monocyclopentadienyl (half-sandwich) complexes - synthesis and structures of allyl complexes - arene complexes - synthesis - structure and reactivity of arene complexes - multidecker complexes.

Unit - V

Organometallic compounds in homogeneous catalytic reactions - coordinative unsaturation - acid-base behaviour reaction - migration of atoms or groups from metal to ligand - insertion reaction - reactions of coordinated ligands - catalytic reactions of alkenes - isomerisation of alkenes - hydrogenation - hydroformylation and hydrosilation of alkenes - alkene polymerisation and oligomerisation - fluxional molecules - The Nobel Prize in Chemistry 2001- Asymmetric synthesis, 2005- Olefins metathesis in organic synthesis and 2010 – Palladium catalysed cross coupling reactions in organic synthesis.

References

1. Organometallics 1, complexes with transition metal-carbon -bonds, Bockmann, Oxford science publications, Oxford, 1996.
2. Organometallics 2, complexes with transition metal-carbon -bonds, Bockmann, Oxford science publications, Oxford, 1996.
3. Basic organometallic chemistry, J. Haiduc and J. J. Zuckerman, Walter de Gruyter, Berlin, 1985.
4. Inorganic Chemistry - Principles of structure and reactivity, J. E. Huheey Harper International Edition, Harper and Rone New York, 1978.
5. Advanced Inorganic Chemistry, F. A. Cotton and G. Wilkinson, Fourth Edition.

CORE XII

Subject Title: PHYSICAL CHEMISTRY – III

(CLASSICAL AND STATISTICAL THERMODYNAMICS)

Course No. 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 the thermodynamics.

Objectives:

On successful completion of the course the students learnt about the fundamentals process involved in 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.

Definition of activity. Activity coefficient. Temperature coefficient of activity. Standard states. Application of activity concept to solutions. The rational and practical approaches. Measurement of solvent activity from colligative properties. Determination of activity of solute. Use of activities in the formation of reaction potentials.

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

Theories of permutations and combinations. Laws of probability. Distribution laws. Gaussian distribution.

UNIT – III : Quantum statistics

Maxwell-Boltzmann statistics. Thermodynamic probability. Thermodynamic probabilities of system in equilibrium. Boltzmann expression for entropy. Sterlings approximation. State of maximum thermodynamic probability. Legrangian multipliers. Thermodynamics probabilities of systems involving energy levels. Maxwell-Boltzmann distribution law. Evaluation of alpha and beta in M-B distribution law.

UNIT – IV :

Partition function – definition, justification of nomenclature, microcanonical and canonical ensembles. Molecular partition function and canonical partition function. The relation between the total partition function of a molecule and the separate partition functions. Translational and rotational partition functions. Effect of molecular symmetry on rotational partition function. Ortho and para hydrogen. Vibrational partition function. Electronic partition function. Evaluation of thermodynamic properties E, H, S, A, G, C_v and C_p from monoatomic and diatomic ideal gas molecule partition functions. Thermodynamics properties of polyatomic ideal gases. Calculation of equilibrium constants for reactions involving ideal gases from partition functions.

UNIT – V : Heat capacities of Solids:

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

Bose-Einstein and Fermi-Dirac Statistics:

Bose-Einstein distribution law. Entropy of Bose-Einstein gas. Planck distribution law for black body radiation – Fermi-Dirac distribution law. Entropy of a Fermi-Dirac gas. Heat capacity of electron gas and the heat capacity of metals. Helium at low temperature. Negative absolute temperature.

References:

1. F.T. Wall – Chemical Thermodynamics, Freeman and Company (1965).
2. S.Glasstone – Thermodynamics for Chemists, Van Nostrand (1964).
3. J.F.Lee, F.W.Sears and D.L.Turcotte – Statistical Thermodynamics (1972)
4. M.C.Gupta – Statistical Thermodynamics, Wiley Eastern Ltd., (1990)
5. G.W.Castellan – Physical Chemistry (1971).

Subject Title : **PAPER IV-INDUSTRIAL CHEMISTRY-IV
(NEW ENERGY SOURCES FOR THE NEW CENTURY, DRUG CHEMISTRY)**
Course Number : **CHMA43D** **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 “Chemistry what is in day today life”.

Objective:

On successful completion of the course the students should have:
Understood what presents in the environment
How to overtake the problems through the environment
Learnt the awareness of forbid newer diseases
Learnt the knowledge of drugs chemistry.

UNIT-1

POLLUTION-ENVIRONMENTAL ISSUE: The air we breathe-composition of air-burning of hydrocarbons-fo-airquality-ozone-oxygen/ozone screen-biological effect of UV radiation-ozone formation and distribution in the atmosphere-paths of ozone destruction-chlorofluorocarbons and their interactions with ozone.

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.

Solar Energy-Fuel from sunlight-splitting of water-hydrogen from sunlight-hydrogen economy-fuel cells-batteries-photovolataics-stealing the sun.

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-Chicken-guinea; 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; Advers Environmental effects of pesticides.

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

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

REFERENCES

- 1) Chemistry in Context: Applying Chemistry to Society, Conard L. Stanitski. Luey Pyrde Eubenks. Catherine H. Middle Camp and Wilmer J. Stratton, third edition, **2000**, Mc Graw Hill.
- 2) Chemistry of the environment, Bailey, Clark, Ferris, Isrause, Strong, second edition, **2001**, Elsevier publications.
- 3) Energy resources and the environment, V. K. Prabhakar, **2001**.
- 1). Fundamental Concepts of Applied Chemistry, Jayashree Ghosh, S.Chand, **2005**
- 2). I. P. Singh, S. B. Bharate and K.K.Bhutani, Current Science, Vol. 89, NO. 2, 25, JULY-**2005**.
- 3). A. Brigo, K. W. Lee, F. Fogolari, G. I. Mustata and J. M. Briggs.
- 4). L.Zhuang *et al.*, *J. Med. Chem.* **2003**, *46*, 453-456.
- 5). D. Sriram *et al.*, *J Pharm Phaemaceut Sci*(www.cspsCanada) 8(3): 565-577, **2005**.

SUPPORTIVE COURSES FOR OTHER DEPARTMENT STUDENTS:

SUPPORTIVE – I

Subject Title: CHEMISTRY IN CONTEXT (APPLYING CHEMISTRY TO SOCIETY)

Course Code: CHMGS10

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 ecological systems

Objectives: After completion of the course the students should have understood biological effects ,energy sources and plastics.

Contents

Unit - I

The air we breathe - composition of air - burning of hydrocarbons - fog - air quality - ozone - oxygen / ozone screen - biological effect of UV radiation - ozone formation and distribution in the atmosphere - paths of ozone destruction - chlorofluorocarbons and their interactions with ozone - the Antarctic ozone hole.

Unit - II

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.

Unit - III

Solar energy - fuel from sun light - splitting of water - hydrogen from sunlight - hydrogen economy - fuel cells - batteries - photovoltaics - stealing the sun - nuclear energy - nuclear fission and fusion - production of electricity by a nuclear reactor - radioactivity and the hazards of radioactivity - living with nuclear power.

Unit - IV

The world of plastics and polymers - polymers - polyethylene - plastics and recreation - paper or plastics - disposal of plastics.

SUPPORTIVE – II

Subject Title: CHEMISTRY IN DAY TO DAY LIFE

Course No. CHMA102GS

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 industrial preparations.

Contents

Unit - I

Carbohydrates - classification - proteins - lipids - nucleic acids and vitamins - sources - applications and diseases due to deficiency.

Unit - II

Fertilisers - classification - characteristics and uses - pesticides and insecticides - a brief study of additives use and abuse of additives in foods and beverages.

Unit - III

Dyes - classification based on mode of application and structure - paints - ingredients - drying - pigments - types and properties - varnish.

Unit - IV

Soaps and detergents - classification - ingredients - solids and liquids - disinfectants (phenyl, dettol type) - perfumes - raw materials - perfumes used in soaps - cosmetics and agarbatti.