DEPARTMENT OF CHEMISTRY

BHARATHIAR UNIVERSITY: COIMBATORE – 641 046.

M.Sc. Chemistry – 2017-2018 onwards

Under choice based credit system (CBCS)

Sl. No.	Credit/Marks	Paper Code	General Title	Specific Title of the paper
			Semester I	
1.	4/100	CHMA13A	Organic Chemistry-I	Reaction Mechanisms
2.	4/100	CHMA13B	Inorganic Chemistry-I	Coordination Chemistry
3.	4/100	CHMA13C	Physical Chemistry-I	Electro Chemistry & Photo Chemistry
4.	4/100	CHMA1EA	Elective – I	Physical methods in chemistry
5	4/100	CHMA1EB	Elective - II	Water treatment and Polymers
6	4/100	CHMA13P	Practicals-I	Organic Practicals
7	2/50	GS06	Supportive-I	Chemistry in Context

			Semester II	
8	4/100	CHMA23A	Organic Chemistry –II	Natural Products, Proteins, and Stereochemistry
9	4/100	CHMA23B	Inorganic Chemistry-II	Bio Inorganic chemistry
10	4/100	CHMA23C	Physical Chemistry II	Quantum Chemistry and Electrochemistry
11	4/100	CHMA2EA	Elective-III	Inorganic spectroscopy
12	4/100	CHMA2EB	Elective - IV	Energy, Diary and Drug chemistry
13	4/100	CHMA23P	Practicals-II	Inorganic Practicals
14	2/50	GS73	Supportive-II	Chemistry in Day- to-day Life

			Semester III	
15	4/100	CHMA33A	Organic Chemistry-III	Organic Photochemistry & Spectroscopy
16	4/100	CHMA33B	Inorganic Chemistry- III	Solid state and Nuclear chemistry
17	4/100	CHMA33C	Physical Chemistry-III	Chemical kinetics surface chemistry
18	4/100	CHMA3EA	Elective-V	Bio Organic Chemistry
19	4/100	CHMA3EB	Elective-VI	Industrial Organic Chemistry
20	4/100	CHMA33P	Practicals -III	Physical Chemistry Practicals
21	2/50	GS	Supportive III	Chemistry of Environment

			Semester IV	
22	4/100	CHMA43A	Organic Chemistry-IV	Aromaticity, Alkaloids, Steroids and Organic structure
23	4/100	CHMA43B	Inorganic Chemistry-IV	Organometallic Chemistry
24	4/100	CHMA43C	Physical Chemistry-IV	Thermodynamics (Classical and statistical)
25	4/100	CHMA43D	Analytical Chemistry	Analytical methods and Techniques
26	8/200	CHMA4LV	Project work	…….

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

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 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 Nnucleophilic 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_N1, S_N2, S_Ni 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(Vilsmeyer- 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 rection) - haloalkylation - aminoalkylation and amido alkylation - 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 conjucated 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-Pondorf 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 - Chugaev 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, $Hg(OAc)_2$, and Pb(OAc) . 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

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. Muk herji 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 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 symmerty - trigonal prism - geometrical isomerism in octahedral complexes - 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 - Addition 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: **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:

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 - Electrolytic conductance – Kohlrausch's law and its applications; ionic equilibria; conductometric and potentiometric titrations.

Unit – II ELECTROCHEMISTRY - II

Metal/Electrolyte interface**:**

Outer Helmholtz plane (OHP) and Inner Helmholtz plane (IHP) - potential profile across double layer region - potential difference across electrified interface - Structure of the double layer - Helmholtz-Perrin, Gouy-Chapman, and Stern models – Electrode kinetics - Butler-Volmer equation–one step one electron transfer kinetics - exchange current density - Tafel equation and plots - Polarizable and non-polarizable interfaces - Hydrogen overpotential – Theories of hydrogen overvoltage - Mechanism of hydrogen evolution reactions - Passivity – electrochemical corrosion and its protection.

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

Absorption and emission of radiation – Theories – Spontaneous and induced emission –Laser – Franck Condon principle - Type 1 & 2 – Physical properties of electronic excited state – Jablonski diagrams – Emission – Resonance emission – Selection rule – Fluorescence – Phosphorescence – Delayed fluorescence: E-Type and P-Type – Excimer and Exciplex complex formation – Stern-Volmer equation – Photosensitization and Chemiluminescence – Experimental techniques – Actinometry – Chemical actinometry – Biochemiluminescence – Photochromism – Photostabilization – Photosynthesis – PS I and PS II – Photochemical energy-storage reactions.

Unit – V COLLOIDS AND CHEMISTRY IN NANOSCIENCE & NANOTACHNOLOGY

Types of solutions – Types of colloidal solutions – Preparation of colloidal solutions – Condensation methods – Disintegraton methods – Purification of colloidal solutions – Dialysis – Ultrafiltration – Characteristics of colloidal solutions – Emulsions – Micelles.

Nanomaterials – Preparation: Plasma arcing - Chemical vapor deposition – Sol-gel method – silica gels – Zirconia and ytrrium gels – Aluminosilicate gels – Electrodeposition – Ball milling –Applications of nanomaterials – Machine tools – Batteries – High power magnets – Motor vehicles and aircraft – Medical applications.

References

1. Samuel Glasstone, "An Introduction to Electrochemistry", Maurice Press, 2007.
2. Gordon M.Barrow-Physical Chemistry,Mc Graw Hill Publishing Company Ltd, 2007.
3. John O'M. Bockris, Amulya K. N. Reddy, "Modern Electrochemistry", Vol. I and II, Plenum Publishing, 2008.
4. Rohatgi Mukherjee K.K.,"Fundamentals of photochemistry", New Age International Pvt. Ltd., New Delhi, 2009.
5. Charles Kutal, Journal of Chemical Education 60 (1983) 882-887.
6. Atkins P.W., "Physical Chemistry", Oxford University Press, 8th edition, 2006.
7. Michael Wilson, Kamali Kannangara, Geoff Smith, Michelle Simmons and Burkhard Raguse, "Nanotechnology – Basic Science and Emergin Technologies", Chapman & Hall (CRC), 2004.

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

General introduction to electromagnetic spectrum – The rotation of molecules – Classification of rotors – Rigid rotors, Non-rigid rotors – Effect of isotopic substitution on the transition frequencies – diatomic and polyatomic molecules – Relative intensities of spectral lines – stark effect – Nuclear and electron spin interaction – Instrumentation – Chemical analysis by microwave spectroscopy.

Unit – II VIBRATIONAL SPECTROSCOPY

Simple harmonic oscillator – Vibrational motion of a diatomic molecule – Selection rule – Zero point energy – Force constant and bond strengths - Anharmonic oscillator - Vibrations of polyatomic molecules – Fundamental vibrations and overtones – Hot bands – Vibrational-rotational spectra of a diatomic molecule – Vibrations of polyatomic molecules - Instrumentation –Sampling techniques - Factors influencing vibrational frequencies - Application to organic and inorganic compounds - Finger print region - Identification of functional groups - Simple problems in functional group identification using IR spectrum.

Unit – III

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:

Structure of atoms – Electronic angular momentum – many-electron atoms – photoelectron spectroscopy and X-ray fluorescence spectroscopy – Zeeman effect – Influence of nuclear spin – problems.

Unit – IV ULTRAVIOLET AND VISIBLE SPECTROSCOPY

Electronic spectroscopy of molecules - Electronic spectra of diatomic molecules - Physical principles – Chromophores and auxochromes - Laws of absorption – Absorption transitions - Instrumentation - Solvent effects - Applications of UV spectroscopy - Effects of conjugation -Woodward-Fieser rules - α,β-Unsaturated carbonyl compounds, dienes trienes and polyenes - Aromatic systems with extended conjugation – Heteroaromatic compounds - Simple problems – Absorption spectra of charge transfer complexes.

Unit – V RADIATION CHEMISTRY AND MORPHOLOGICAL STUDIES:

Radiation chemistry: Source of high energy – interaction of high energy radiation with matter – primary and secondary process –G-value –radiolysis of water – reactions of hydrated electrons OH and H radicals – experimental techniques (Dosimetry).

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

References

1. Banwell C. N., "Fundamentals of Molecular Spectroscopy", Tata McGraw-Hill Publishing Company Limited, New Delhi, 4th Edition, 2004.
2. Chang - Basic principles of spectroscopy.
3. Donald L. Pavia, Gary M. Lampman and George S. Kriz, Jr - Introduction to Spectroscopy: A Guide for students of organic chemistry.
4. D.H.Williams-Ian Fleming, Spectroscopic Methods in Organic Chemistry,Mc Graw Hill Publishing Company Ltd, 2006.
5. G. Friedlander, J.W. Kennedy and J.M. Miller, Nuclear and Radiochemistry, Wiley, 1964.
6. Zhou W, Wang Z. L, "Scanning Microscopy for Nanotechnology: Techniques and Applications", Springer, New York, USA, 2006.

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 H_2O and D_2O.

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 (10^{th} Edition, 1999)
2. *Outlines of Chemical Technology* – For the 21^{st} Century – M.Gopala Rao & Marshall Sittig (3^{rd} Edition, 1997)

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) Acetylsalicyclic acid from salicyclic acid
   (iv) 2,4,6-Tribromoaniline from aniline
   (v) p-Bromoacetanilide 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

Polymers –Introduction-Definition- Types of polymers based on physical property-Characteristics of polymers- polyethylene – PVC- Synthetic fibres –Definition, Nylon 66, and Terelene.

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:

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 proteins.

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 - perhydrophenantharene - decalins - carbohydrates - spiranes- allenes and biphenyls.Asymmetric Synthesis-Introduction-methods of asymmetric synthesis-auxiliary controlled methods-reagent controlled methods-catalyst controlled methods.

Unit - IV

Vitamins:

Structure and synthesis of vitamin B complex : vitamin B_1 (aneurin) - vitamin B_2 (riboflavin) - pantothenic acid - folic acid - vitamin H (biotin) - vitamin B_6 (pyridoxine) - vitamin B_{12} (cyanocobalamin) structure only - vitamin E (Alpha - tocopherol) - vitamin K_1 (phylloquinone) and vitamin K_2.

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, oxitanes and thietanes.

b) Benzo fused Heterocycles – benzofurans, benzothiophenes, carbazole - chromone - flavanones - flavones - flavonols – isoflavones.

References

1. I. L. Finar, Organic chemistry, vol. I and vol. II.
2. Nakanishi et. al., Natural product chemistry, vol. I, Academis press, 1974.
3. Newman, Terpenes and Terpenoids.
4. E. L. Eliel, Stereochemistry of carbon compounds, Mc Graw Hill, 1962
5. P.Ramesh, Basic principles of Organic Stereochemistry,Meenu publication,2005.
6. Heterocyclic Chemistry, J. A. Joule, K. Mills and G. F. Smith, Chapman and Hall
7. Heterocyclic Chemistry, T. L. Gilchrist, Longman Scientific Technical
8. R. K. Bansal, Heterocyclic Chemistry; 3rd Ed., Wiley Eastern Ltd, New Delhi, 1999.

CORE V

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 B_{12} 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:

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.
3. J.E.Huheey, E.A.Kieter, R.L.Keiter, Inorganic Chemistry 4th Edition, Addision Wesely Publishing Company.
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.

Electron spin and the Pauli principles – symmetric and antisymmetric nature of the wave functions - Slater determinants - approximate wave function of many electron atoms - Born Oppenheiner approximation - Elementary concepts of MO and VB theories - Hybridization – Huckel theory of linear conjugated systems – Cyclic systems – Wood-ward Hoffman rules.

Unit – IV 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 - Statement and proof of Great Orthoganality 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_2O, NH_3, BF_3) - Selection rules for vibrational spectra – IR and Raman active fundamentals – Mutual exclusion rule - Symmetries of M.O and symmetry selection rule for electronic transition in ethylene and formaldehyde - Hybridization schemes for atoms in ethylene and butadiene.

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. Swarnalakshmi S. - A Simple Approach to Group Theory in Chemistry, Universities Press, 2009.
8. Raman, K.V. - Group theory and its applications to chemistry", Tata Mac Graw Hill, 2004.

9 . F. A. Cotton – Chemical applications of group theory, Wiley India Pvt Ltd 3rd Edn,, 2008.

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

ESR introduction - Zeeman Equation, g-value, nuclear hyperfine splitting - interpretations of the spectrum, simple carbon centered free radicals. Anisotropy-g-value and hyperfine splitting constant - McConnel's equation - Krammer's theorem – spin-orbit coupling – dipolar contribution – dipole-dipole interaction - ESR of transition metal complexes (copper, manganese and Vanadyl ions) – isotropic, axial and rhombic spectra of copper(II) systems – Application of EPR: Structural elucidation of coordination complexes: Determination of electron delocalization, bonding mechanism of dioxygen adducts of dinuclear cobalt complexes, determination of nuclear spin state – EPR of low-spin Hemes, blue copper proteins.

Unit-IV - Inorganic NMR, NQR spectroscopy

^{31}P , ^{19}F NMR spectrum of HPX_2, P_4S_3, TiF_4, BrF_5, SF_4, SF_6, XeF_4O, C SIF_6^{2-}, $B_3H_8^-$, NF_3, $P_3N_3Cl_4F_2$, 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 - Mossbauer 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: Mossbauer spectra of high- and low-spin iron compounds and tin halides systems: Prussian blue-Turn bulls blue, iron-carbonyl compounds,

Sodium nitroprusside, FeX_2, SnX_4, SnX_6, SnX_5Y (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.

X-ray absorption spectroscopy (XAS) and Extended X-ray absorption fine structure (EXAFS) – Applications of X-ray absorption spectroscopy. X-ray Absorption Edges - X-ray Fluorescence - Measurement of X-ray Absorption Spectra -Theoretical Description of EXAFS Spectra - Single scattering, Multiple scattering – Data reduction and analysis - Applications: structure determination, Resolution of crystallographic disorder, Oxidation state, prediction of molecular symmetry, determinations of atoms present in the first coordination sphere (Edge & EXAFS analysis) – Structure of Metal clusters.

References

1. Lawrence Que, Jr, Physical Methods in Bioinorganic Chemistry
2. Russell S Drago , Physical methods in Inorganic Chemistry
3. I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, Bioinorganic Chemistry; University Science Books .
4. Asim K Dass, Bioinorganic Chemistry.
5. E. I. Solomon and A. B. P. Lever, Inorganic Electronic Structure and Spectroscopy
6. E.A.V Ebsworth, Dawid W. H. Rankin and Stephen Cardock, Structural methods in Inorganic chemistry.
7. David W. H. Rankin, Norbert W. Mitzel, Carole A. Morrison, Structural Methods in Molecular Inorganic Chemistry.

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

POLLUTION-ENVIRONMENTAL ISSUE: The air we breathe-composition of air-burning of hydrocarbons- 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.

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-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; Nitrogeneous 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

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**.

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

5). I. P. Singh, S. B. Bharate and K.K.Bhutani, Current Science, Vol. 89, NO. 2, 25, JULY-**2005**.

6). A. Brigo, K. W. Lee, F. Fogolari, G. I. Mustata and J. M. Briggs.

7). L.Zhuang et al., J. Med. Chem. **2003**, 46, 453-456.

8). D. Sriram et al., J Pharm Phaemaceut Sci(www.cspsCanada) 8(3): 565-577, **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 commerical 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

Fertilizers – Pesticides - Insecticides – Definition, Classification, Characteristics and Uses. Additives –Definition, Characteristics, Uses and Abuse of additives in foods and beverages.

Unit - III

Dyes – Definition, Classification based on mode of application and structure, Applications. Paints – Definition, Ingredients, Characteristics, uses and drying process. Pigments -Varnishes - Definition, Characteristics, Types and Uses.

Unit - IV

Soaps and Detergents - Definition, Ingredients, Classification, Characteristics and Uses. Disinfectants – Definition, Characteristics and Uses. Perfumes - Definition, Characteristics, Raw materials and perfumes used in soaps - Cosmetics.

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}C NMR (elementary idea only).

Applications of organic spectroscopy:

Structure determination of organic compounds by using UV-Vis, IR, ^{1}H & ^{13}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:

Light absorption – Experimental techniques – Electronic transitions – Franck – Condon principle – Jablonski diagrams – Intersystem crossing – Energy transfer – Molecular orbital view of excitation – The geometry of excited states – Reactivity of electronically excited ketones –alpha - cleavage - gamma - hydrogen transfer Norrish Type I, Type II, Type III reactions – Photoreduction – Oxetane formation – Reactivity of Pi, Pi* excited ketones – Photochemistry of alpha, beta - unsaturated ketones – Optical pumping – Dienone phenol rearrangement.

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:

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. R. M. Silvertein and G. C. Baseler - Spectroscopic identification of organic compounds.
2. Donald L. Pavia, Gary M. Lampman, and George S. Kriz, Jr - Introduction to Spectroscopy : A Guide for students of organic chemistry.
3. William Kemp - Organic spectroscopy.
4. Photochemistry in Organic Synthesis – edited by J.D. Coyle – Royal society of Chemistry 1986.
5. Photochemistry of heterocyclic compounds – Ole Buchardt – Wiley Interscience 1976.
6. Molecular Photochemistry N.J.Turro and W.A. Benjamin.
7. Molecular reactions and Photochemistry - Charles H.Depuy, Orville.S. Chapman, Prentice – Hall of India Pvt., Ltd. 1988.
8. Frontier orbitals and organic chemical reactions - Ian Fleming John Wiley and sons, 1976.

CORE VIII

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

Types of solids - close packing of atoms and ions - bcc , fcc and hcp voids - radius ratio - derivation - its influence on structures - structures of rock salt - cesium chloride - wurtzite - zinc blende - rutile - fluorite - antifluorite - 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.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
8. H.J.Arnikar – Essentials of Nuclear chemistry.

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

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 hardsphere collision theory – Thermodynamic formulation-activated complex theory (Enthalpies and entropies of activation) – Kinetic isotopic effect.

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.

Surface Phenomenon and Heterogeneous catalysts - Adsorption and free energy relation at interfaces – Gibbs adsorption isotherm – Physisorption and chemisorptions – Adsorption isotherms (Langmuir and BET) – Measurement of surface area – Kinetics of heterogeneous catalysis (Langmuir hinshelwood mechanism and Eley-Rideal mechanism) – Semiconductor catalysis.

Unit - V 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.

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.

ELECTIVE V

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 reterosynthesis - 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 acylic 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-NH_2 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:

Design, development and mechanism of action of drugs: Antimicrobial, anticancer, antidiabetic, antiinflammatory and antitubercular drugs and their mechanism of action. Cardiovascular drugs: Cardiotonic, Antihypertensive, Antirhythmic and Lipotropic drugs.

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

References

1. Organic Synthesis, 2nd Edition by Michael B Smith, McGraw-Hill, New York.
2. R.K. Mackie and D.M. Smith. 1998, Guide book to organic synthesis, ELBS Publication.
3. I. L. Finar, 1986, Organic Chemistry, 5th Edition, Vol .II, ELBS Publication.
4. L. Smith, Robert L. Hill .1. Robert Lehman, Robert J .Iet Rowitz, Philp Handler and abrahim white principles of Biochemistry General aspects, 7th Edition, McGraw Hill Int.
5. L. Stryer, Biochemistry, W.H.Freeman and Co., New York.
6. http://www.cuchd.in/e-library/resource_library/university%20institutes%20of%20sciences/Fundamentals%20of%20Biochemistry/Chap-20.pdf.
7. B.l. Smith, 1980, Organic synthesis, Chapman and Hall, NY.
8. Francis.A. Carey, Richard J. Sundbreg, 2001, Advanced Organic Chemistry, 4th Edition, Plenum Press, New York.
9. Medicinal Chemistry for the 21st Century. Ed. C. G. Wermuth, Blackwell, Oxford, 1992, ISBN 0632034084.
10. Drug Metabolism: Databases and High Throughput Testing During Drug Design and Development. Ed. P. W. Erhardt, Blackwell, Oxford, 1999. ISBN 0632054329.
11. Heterocyclic Chemistry, J. A. Joule, K. Mills and G. F. Smith, Chapman and Hall.
12. Heterocyclic Chemistry, T. L. Gilchrist, Longman Scientific Technical.

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:

Introduction-raw materials-saturated hydrocarbons from natural gas-uses of saturated hydrocarbons-unsatutated 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-iodine value-wijs method-Reichert meissl 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-themoplastic and thermosetting polymers-phenolic resins,poyurethanes,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 (10^{th} Edition)
2. *Outlines of Chemical Technology* – For the 21^{st} Century – M.Gopala Rao & Marshall Sittig (3^{rd} 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 kinectics,conductivity and potentiometric titrations.

Goals:
To motivate the students to understand the principles of chemical kinectics,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.**

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. Validition 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 commerical 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

Milk- Composition of milk-Properties of milk- Effect of heat on milk- Pasteurisation: Definition, process and its effects- Homogenisation- Milk products- Ice cream.

Unit - IV

Introduction- Oils- Definition, Classifications, Properties, and uses- Animal, Vegetable and Mineral oils- Fat-Definition- Functional properties- Types of Fat- Uses- Effect of fat on health.

CORE X

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:

Aromaticity- Concept of aromaticity – aromaticity of benzenoid and non benzenoid compounds – effect of aromaticity on bond lengths – resonance – resonance energies – electronic absorption spectra and induced ring currents – Huckel‟s rule – structure and synthesis of azulenes – ferrocenes – sydnones – tropolones – fulvenes – annulenes.

Green Chemistry:

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

Unit – II

Alkaloids:

Structural elucidation and biosynthesis of dictamnine – chinconine – morphine – reserpine – aeronycine – cocaine – lysergic acid and nicotine.

Unit - III

Steroids:

Structural elucidation and spectrum of cholesterol – erogosterol - vitamin-D – equilenin – estrone - progesterone, Stigmasterol, Steriod harmones, androsterone, testosterone, Oesterol, Oestradiol, biosynthesis of steroids – Structure - synthesis of bile acids.

Unit – IV

Named reactions:

Baylis-Hillman reaction, Mannich, Simmons – Smith, Reformatsky, Ullmann, Wittig–Horner, Peterson, Acyloin condensation, Robinson annulations, Oppenauer oxidation, m-ClC_6H_4COOOH.

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, $LiAlH_4$, Ozone, OsO_4, DCC, 1,3-Dithiane, LTA, Peracetic acid, Raney Nickel, PPA, CH_2N_2, Tri-n-butyl tin hydride, *n*-Butyl lithium, NBS, DDQ, DBU (Diaza bicyclo-undecane), SeO_2, Tri methyl silyl iodide, Gilman's reagent, 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, Steriods, Reinbold, 1959.
4. P.J.Garrat, Aromaticity, Mc Graw Hill, 1971.
5. Jerry March Advanced Organic Chemistry.
6. R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, Organic Chemistry, 7th Edition, Pearson Education.
7. P. Y. Bruice, Organic Chemistry, 4th Edition, Pearson Education.
8. T. W. Graham Solomons and C. B. Fryhle, Organic Chemistry, 10th edition, Wiley.
9. Fieser & Fieser – Reagents in Organic Synthesis.

CORE XI

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

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 – Wade's 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 - Cp_2Fe/Cp_2Fe^+ 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- Assymetric 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, Brelin, 1985.
4. Inorganic Chemistry - Priciples 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 – 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.

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 STATISTICAL THERMODYNAMICS - I

Maxwell-Boltzmann statistics – Thermodynamic probability – Thermodynamic probabilities of system in equilibrium – Boltzmann expression for entropy – Sterling's 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: STATISTICAL THERMODYNAMICS - II

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, Cv and Cp from monoatomic and diatomic ideal gas molecule partition functions – Thermodynamics properties of polyatomic ideal gases – Calculation of equilibrium constants of reactions involving ideal gases from partition functions.

Unit – V: STATISTICAL THERMODYNAMICS - III

Bose-Einstein and Fermi-Dirac Statistics:

Bose-Einstein distribution law – Entropy of Bose-Einstein gas -Plank 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.

Heat capacities of Solids:

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

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.Turcottee – Statistical Thermodynamics (1972)
4. M.C.Gupta – Statistical Thermodynamics, Wiley Easter Ltd., (1990)
5. G.W.Castellan – Physical Chemistry (1971).

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

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’-teat, ‘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 – Eletrothermal 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), 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:

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.