

DEPARTMENT OF CHEMISTRY

B.Sc. (Special) - Chemistry Course Content - 2019 Batch

CHE1201FP VOLUMETRIC ANALYSIS (LAB)

LEARNING OUTCOME :

4 hrs./wk.

On successful completion of the course, the student will be able to

- acquire knowledge on lab safety and precautionary measures
- develop the skills for handling glasswares
- use different concentration units to prepare standard solutions
- analyze and estimate a chemical substance using titrimetric principles

COURSE CONTENT :

60 hrs

- Lab ethics and safety measures in a chemical laboratory
- Handling electronic analytical balance
- Calibration of volumetric glasswares
- Basic Concepts : Discussion and Problem solving – Equivalent weight of acids, bases, oxidizing and reducing agents – Normality– Molarity– Molality– ppm– percent solution – Saturated unsaturated and supersaturated solutions.

EXPERIMENTS:

1. Preparation of standard solutions and dilutions
2. Estimation of sodium hydroxide
3. Estimation of acetic acid
4. Estimation of Fe (II) / Fe(III) in a mixture
5. Estimation of copper by Iodometry
6. Estimation of iron by Permanganometry
7. Estimation of magnesium by Complexometry
8. Estimation of chloride by argentometric titration
9. Estimation of Calcium by indirect method

REFERENCE BOOK(S)

Day R A., Underwood A I.,(1991). *Quantitative Analysis*, 6th ed., New York : Pearson Emory University. Print.

Jeffery G.H., Bassett J., Mendham J., and Denney R.C.,(1989). *Vogel's Textbook of Quantitative Chemical Analysis*, 5th ed, New York : Longman Scientific & Technical. Print.

CHE1402CM GENERAL CHEMISTRY (Theory)

LEARNING OUTCOME :

5 Hrs./Wk.

- On successful completion of the course, the student will be able to
- correlate the structure and behaviour of atom

- analyze and interpret the gradation in the properties of elements in the periodic table
- differentiate the various chemical interactions in molecules through bonding concepts
- predict the nuclear transmutations
- identify the role of radioactive materials in different applications.

COURSE OUTLINE :

UNIT-I : STRUCTURE OF ATOM

15 Hrs.

Discovery of electron - measurement of e/m for electrons - determination of charge on an electron - positive rays - protons, neutrons - sub-atomic particles, alpha particles, Rutherford's atomic model - Mosley's determination of atomic number - mass number - quantum theory of electromagnetic radiation - photoelectric effect and Compton effect - Bohr theory of hydrogen atom - spectrum of hydrogen atom - The Sommerfield's extension of Bohr's theory.

UNIT-II : PERIODIC TABLE AND ATOMIC PROPERTIES

15 Hrs.

The long form of periodic table - Electronic configuration of atoms - Division of elements - Cause of periodicity - Periodicity of Atomic properties - Covalent, van der Waal's and ionic radii - Ionisation energy, electron affinity and electronegativity - factors affecting the periodic properties - determination of electronegativity - Pauling's approach, Allred and Rochow's approach, Mulliken's approach - Applications of electronegativity.

UNIT-III : CHEMICAL BONDING –LEWIS CONCEPT

15 Hrs.

Chemical bond - types of bonds - ionic bond - factors favoring the formation of ionic compounds, Born-Haber cycle - properties of ionic compounds - electrovalency, covalency, variable valency - factors favouring the formation and properties of covalent compounds - comparison of ionic and covalent compounds - octet rule and failure of octet rule - polar and non polar covalent bonds and molecules - transition from ionic to covalent character - Fajans' rule - applications of Fajan's rule - coordinate bond - Properties of coordinate compounds - comparison between ionic, covalent and coordinate bonds - metallic bond - properties of metals - hydrogen bonding - types – consequences of hydrogen bonding - importance of hydrogen bonding in sustaining life. Types of intermolecular interactions - electrostatic and van der Waals interactions.

UNIT-IV : CHEMICAL BONDING – ORBITAL CONCEPT

15 Hrs.

Linnett's DQ theory - VSEPR theory - VBT of covalent bond - formation of sigma and pi bonds - Resonance structures of CO, CO₂, CO₃²⁻, O₃, SO₂, SO₃ - hybridisation - sp, sp², sp³, sp³d, sp³d² hybridisation - Molecular orbital theory - LCAO method - bonding and antibonding orbitals - formation of MOs in homonuclear and heteronuclear diatomic molecules and ions.

UNIT-V : NUCLEAR CHEMISTRY

15 Hrs.

Composition of nucleus - nuclear size - nuclear forces - packing fraction - nuclear density – mass defect - binding energy of the nucleus - nuclear models - nuclear shell model - concept of nuclear spin-liquid drop model - collective model.

RADIOACTIVITY - Rays from radioactive materials - range of alpha particles – radioactive disintegration - radioactive decay and half life - Geiger - Nuttal rule - radioactive equilibrium - steady state - transmutation of elements - group displacement rule - nuclear stability – radioactive series - applications of radioactivity - isotopes - isobars - isotones - separation of isotopes - Determination of atomic masses - mass spectrographs - artificial radioactivity - induced radioactivity - transuranic elements - nuclear coulombic energy barrier - cyclotron - synchrocyclotron – linear electron accelerator

- Q- values of nuclear reactions - Nuclear fission - The fission chain reaction - release of fission energy - uncontrolled and controlled - disposal of radioactive wastes from nuclear reactors - Nuclear fusion - hydrogen bomb - controlled nuclear fusion - fusion in stars – nuclear energy as an alternative energy resource.

TEXT BOOK(S)

Madan R.D., **Modern Inorganic Chemistry**, 3rd edition, New Delhi, S. Chand & Co. Ltd., 2011, Chapters: UNITS II,III&IV.

Puri B.R, Sharma L.R and Pathania S., **Principles of Physical Chemistry**, 46th edition, New Delhi, Vishal Publishing Co., 2012, Chapters: UNITS I & V.

REFERENCE BOOK(S)

ArunBahl, B.S. Bahl and G.D.Tuli, **Essentials of Physical Chemistry**, New Delhi, S.Chand and Co. Ltd., 2009, Chapters: Unit I,II,III,V.

CHE1201FS FUNCTIONAL ENGLISH FOR CHEMISTS

(Theory)

LEARNING OUTCOME :

2 Hrs./Wk.

- On successful completion of the course, the student will be able to
- develop listening skills
- construct, correct and concise grammatical sentences
- identify the appropriate word and improve the vocabulary
- analyze the given passage and draw inferences
- demonstrate oral communication skills

COURSE OUTLINE :

UNIT-I : LISTENING SKILLS

10 Hrs.

Types of Listening - Tips for Effective Listening - academic listening - Listening to Talks in chemistry and Presentations - Comprehension

UNIT-II : WRITING AND SPEAKING SKILLS

10 Hrs.

Parts of Speech - noun - types of noun - verbs - types of tense - the Sentence - the phrase – kinds of sentences - parts of sentence - adjectives - adverbs - preposition – Interjection - conjunction - punctuation marks - articles - paragraph - construction of paragraph - linkage and cohesion - summary - Précis - Writing - notes taking - Report - Abstracts - Letter Writing - Barriers of Communication. Examples and activities will involve chemistry concepts.

UNIT-III : READING SKILLS

10 Hrs.

Importance of reading - types of reading - skimming - scanning - reading for information – technique of reading - SQ3R (S-Survey Q-Question 3R-Read, Recite, Review.) Passages for reading to be selected from Science and technology column (Newspaper) and simple everyday chemistry applications from books.

TEXT BOOK(S)

Nthira S.R. and Saraswathi V, **Enrich Your English Book I: Communication Skills**, Oxford University Press, Oxford, New York.

WEBSITE(S) :

http://depssa.ignou.ac.in/wiki/images/c/ca/Communication_skills_in_English.pdf

<http://eltvoices.in/Volume1/Issue1/EV111.5.pdf>

<http://www.angrau.net/StudyMaterial/English/ENGL101.pdf>

<http://www.sharadavikas.com/SourceMaterials/btc34.pdf>

CHE 2503CM BASICS OF ORGANIC CHEMISTRY

THEORY

LEARNING OUTCOME :

5 hrs./wk.

On successful completion of the course, the student will be able to

- apply the IUPAC rules to name organic compounds
- acquire the knowledge on the basic concepts of reaction mechanisms
- illustrate the mechanisms involved in reactions of alkanes, alkenes, alkynes and alkydienes
- formulate a suitable mechanism for reactions of aliphatic hydrocarbons

COURSE CONTENT :

UNIT-I : NOMENCLATURE OF ORGANIC COMPOUNDS

15 hrs.

IUPAC nomenclature – rules for naming organic compounds: alkanes, alkenes – alkynes – cycli aliphatic hydrocarbons – alkyl halides – alcohols – ethers – aldehydes – ketones – carboxylic acids and its derivatives – alkyl cyanides – nitroalkanes and amines – selected examples of monofunctional and polyfunctional organic compounds– structure of organic compound from its IUPAC name – common errors in writing IUPAC names.

UNIT– II : FUNDAMENTALS OF ORGANIC REACTION MECHANISMS

15 hrs.

Electronic displacements – inductive effect, electromeric effect – mesomeric effect– hyper conjugation– Steric effects – heterolytic and homolytic cleavages – reactive intermediates – carbocations – stability of carbocations – carbanions – stability of carbanions – free radicals – stability of free radicals – carbenes – nitrenes – electrophiles and nucleophiles – types of reactions –substitution – addition – elimination and rearrangement reactions.

UNIT– III : ALKANES AND ALKENES

15 hrs.

ALKANES: Introduction – chemical properties– free radical substitution reactions– halogenation (reactivity and selectivity) nitration– sulphonation– oxidation reactions.

ALKENES: Introduction– physical properties– preparation: reduction of alkynes– elimination reactions– Wittig reaction– Kolbe's electrolytic method – chemical properties– stability of alkenes– electrophilic addition reactions– addition of halogens– hydrogen halide– sulphuric acid – water – oxymercuration– demercuration reaction– hydroboration– peroxyacid– alkenes– carbenes– free radical addition reaction– Addition of HBr(peroxide effect)– oxidation reactions– hydroxylation of alkenes with Baeyer's reagent– acidified and alkaline KMnO_4 – OsO_4 – $\text{K}_2\text{Cr}_2\text{O}_7$ – $\text{Pb}(\text{OAc})_4$ – ozonolysis– allylic substitution reactions – polymerization of alkenes.

UNIT– IV : ALKADIENES

15 hrs.

Introduction– stability of dienes– preparation of buta- 1,3- diene– molecular orbital picture of 1,3-butadiene– Chemical properties of buta-1,3-diene – reduction and oxidation reactions– electrophilic addition reaction(1,2- addition Versus 1,4-addition) –free radical addition reactions– Diels-Alder reaction.

Polymerization– isoprene– preparation– chemical properties– chloroprene– preparation– chemical properties

UNIT-V : ALKYNES

15 hrs.

Introduction– preparation (recall)– physical properties– chemical properties– addition of hydrogen– electrophilic addition reactions oxidation reactions– addition of halogens, hydrogen halides, water– nucleophilic addition reactions– reactions involving acetylenichydrogens– reactions with sodamide, lithium amide and Grignard reagent –synthetic application of metal alkynides– reaction of terminal alkynes with ammoniacal cuprous chloride– silver nitrate– polymerization reactions– isomerization (Acetylenic Allene Rearrangement).

TEXT BOOK(S):

Jain. M. K., Sharma, S. C.,(2013). *Modern Organic Chemistry*, (4th ed.), New Delhi: Vishal Publishing.Print.

REFERENCE BOOK(S):

Bruice. P.Y., (2002). *Organic Chemistry*,(3rd ed.), New Delhi: Pearson education Inc. Print.

Ghosh S.K.,(1998). *Advanced General Organic Chemistry*, (2nd ed.), Calcutta: Books and Allied (P) Ltd. Print.

Mehta B,and Mehta, M., (2011). *Organic Chemistry*, (6th ed.), New Delhi: PHI Learning Private Limited Print.

Morrison R. T, Boyd R.N, and Bhattacharjee S. K.,(2011). *Organic Chemistry*,(7th ed.), New Delhi: Pearson. Print.

Solomons T. W.G., Fryhle C.B.and Snyder S.A.,(2016). *Organic Chemistry*, (11th ed.),United States: Wiley. Print.

CHE 2203CP SEPARATION AND PURIFICATION TECHNIQUES (LAB)

3 hrs. /wk.

LEARNING OUTCOME:

On successful completion of this course, the student will be able to

- employ the techniques for the purification of organic compounds.
- apply the techniques for the extraction of natural products
- use chromatographic techniques for the separation of mixture of compounds

COURSE CONTENT:

45 hrs.

TECHNIQUES FOR SEPARATION AND PURIFICATION:

1. Purification of organic compounds by crystallization using the following solvents:

- a. Water
- b. Alcohol
- c. Alcohol-Water

2. Determination of melting and boiling point

3. Distillation

- a. Simple
- b. Steam
- c. Fractional

4. Soxhlet extraction

5. Solvent extraction technique for separation of organic mixture

6. Chromatographic techniques:

Adsorption Chromatography

- a. Column
- b. TLC

Partition Chromatography

- c. Paper– Ascending
- d. Circular disc

All lab classes will have pre-lab discussions.

REFERENCE BOOK(S):

Donald L Pavia, Gary M. Lampman, George and S Kriz, (2009). *Organic Chemistry – A Lab Manual* New Delhi: Sengage Learning. Print.

Furniss B.S. (1989). *Vogel's Textbook of Organic Chemistry*, (5th ed.), London: ELBS. Print.

CHE2202FS DATA HANDLING AND PRESENTATION

(Theory)

LEARNING OUTCOME :

2 Hrs./Wk.

On successful completion of the course, the student will be able to

- classify the various types of data
- analyze and tabulate the data
- make use of computers to represent the data
- design a scientific report

COURSE CONTENT :

30hrs.

UNIT-I : DATA ANALYSIS

10 hrs.

Data– Definition – Types of data – Categorical or qualitative and numerical or quantitative – Categorical – nominal and ordinal – numerical – discrete and continuous, interval and ratio – Classification of data – chronological, geographical, qualitative , quantitative, frequency distribution– Data collection– Primary and secondary – variable – dependent and independent – accuracy and precision – significant figures – measure of central tendency – mean, median and mode and measures of dispersion – Range, mean deviation, standard deviation

UNIT-II : DATA REPRESENTATION

10 hrs.

Tabulation of data – conversion of table to diagrams and graphs – Diagrams – bar and pie diagram– Graphs – line and frequency distribution – linear graphs (identification of slope and intercept values) – Use of error bars in presenting graphical data – Using computers to prepare tables, spread sheets and graphs .

UNIT-III : REPORT PREPARATION

10 hrs.

Data interpretation – preparation of report – presentation of report (written & oral) – Use of computer in preparation and presentation of a scientific report – use of computer aided tools to represent chemical structures – effective usage of internet for literature search – plagiarism.

TEXT BOOK

Gary D. Christian, (2011). *Analytical Chemistry*, (6th ed.), New York: John Wiley & Sons. Print.

REFERENCE BOOK(S)

Douglas A. Skoog and Donald M. West, F. (2011). James Holler, Stanley R. Crouch, *Fundamentals of Analytical Chemistry*, (9th ed.), United States: Cengage learning. Print.

Jeffery G.H., Bassett J., Mendham J., Denney R.C., (1989). *Vogel's Textbook of Quantitative Chemical Analysis*, (5th ed.), New York: Longman Scientific & Technical. Print.

Nirmala Jeyaraj (ed.td.), (2008). *Introduction to Research Methodology (A multidisciplinary approach)*, Madurai: Lady Doak College. Print.

CHE2201NI ENVIRONMENTAL CHEMISTRY

(Theory)

LEARNING OUTCOME :

2 Hrs./Wk.

On successful completion of the course, the student will be able to

- identify basic environmental contaminants
- recognize the importance of environmental changes
- outline the various control measures
- reflect on burning environmental issues

COURSE OUTLINE :

UNIT I: SEGMENTS OF ENVIRONMENT

7 Hrs.

Atmosphere - composition, particles, ions and radicals in the atmosphere. Hydrosphere – Water resources - Lithosphere - composition of soil, inorganic and organic compounds, micro and macronutrients in soil. Biosphere.

UNIT II: ENVIRONMENTAL POLLUTION

8 Hrs.

Definition, Causes, effects and control measures of (a) Air pollution (b) Water pollution (c) Soil pollution (d) Noise pollution (e) Radioactive pollution. Solid waste management: control measures of urban and industrial wastes, integrated waste management of plastics. Disaster management: Floods, earthquake, cyclone and landslides

Activities

- Analysis of fine particulate matter
- Water analysis
- Discussion and reflection on Role of an individual in prevention of pollution

UNIT III: ENERGY SOURCES AND ENVIRONMENT

8 Hrs.

Classification of fuels and energy sources - conventional (Coal, natural gas, fossil fuel) and non - conventional, renewable and non - renewable energy sources - **geothermal energy** – different types, origin and utilization, **solar energy** - introduction, direct utilization of solar energy as heat energy through collectors - ocean energy, **biomass based energy** - bio gas and gobar gas - special uses of biomass as fuels - **hydropower**.

Activity : Discussion and reflection on Urban problems related to energy

UNIT IV: SOCIAL ISSUES AND ENVIRONMENT

7 Hrs.

Environment Protection Acts - Protocols - Kyoto, Montreal - **Carbon credits** - introduction and significance, **Carbon footprint, Carbon trading** - **Water crisis** - water conservation and rain water harvesting, water recycling - **Wasteland** reclamation - **Consumerism and waste products** - **Energy Crisis** - **Nuclear energy** - fusion vs fission for power generation, threats and challenges.

Activities

- Calculation of carbon and ecological footprint
- Discussion and reflection on Organic Farming-An alternative to fertilizers and pesticides?

Common Activities

- Sensitize the students for energy conservation on campus
- Collection of articles on environmental issues from magazines, newspaper
- On the spot study, Knowing the eco initiatives of campus - visit to vermiculture, paper recycling unit, Herbal garden , incineration unit etc

REFERENCE BOOK(S)

AsimK.Das, **Environmental Chemistry with Green Chemistry**, Kolkata, Book and Allied Pvt. Ltd, 2010.

Bhatia S.C, **Environmental Chemistry**, Newdelhi, CBS publishers, 2002.

Gary W.vanLoon& Stephen J.Duffy, **Environmental Chemistry**, New York, Oxford University Press, 2003.

Sodhi G.S, **Fundamental concepts of Environmental Chemistry**, New Delhi, Narosa Publishing House, 2000.

CHE3504CM ORGANIC REACTION MECHANISM

(THEORY)

LEARNING OUTCOMES:

On successful completion of the course, the student will be able to

- infer the rates of the reactions of alkyl halides using mechanistic details
- apply the reactivity of alcohols, phenols, ethers and epoxides for developing new synthetic methodologies
- identify the aromatic compounds and predict its reactivity and toxicity
- illustrate the mechanism of electrophilic and nucleophilic substitution reactions in aromatic compounds
- explain the reactions of polynuclear hydrocarbons and their applications in day today life

COURSE CONTENT:

5 hrs./wk.

UNIT I: ALKYL HALIDES

15 hrs.

Nomenclature and classification of organic halogen compounds – preparation – Hunsdiecker reaction – Finkelstein reaction – Swart's reaction – halogenation of alkanes – free radical mechanism – reactions of alkyl – vinyl and allyl halides – nucleophilic aliphatic substitution – orientation – kinetics of nucleophilic aliphatic substitution – duality of mechanism – S_N2 & S_N1 reaction – mechanism – kinetics – stereochemistry – reactivity – rearrangement of carbonium ion – elimination – mechanisms: E1 – E2 and E1cB – reactivity – orientation (Saytzeff/ Hofmann) and stereoselectivity – elimination vs substitution.

UNIT II: ALCOHOLS, PHENOLS, ETHERS AND EPOXIDES:**15 hrs.**

Alcohols: Physical properties – alcohols as an acid and as a base – reactions involving the acidic and basic characteristics of alcohols – relative reactivity of 1^o, 2^o, 3^o alcohols and distinction – ascent and descent in alcohol series – comparison of alcohol with thiols.

Phenols: Preparation and properties – acidity and factors affecting it – ring substitution reactions – coupling with diazonium salts – Reimer-Tiemann and Kolbe-Schmitt reaction – Lederer-Manasse reaction – Gattermann synthesis – Houben-Hoesch reaction – Pechmann condensation with mechanism – reactions of analytical importance. Ethers: Preparation – Williamson ether synthesis – alkoxymercuration and demercuration of alkenes – reactions involving ethereal oxygen and ether linkage – comparison of ethers with thioethers – crown ethers (introduction only).

Epoxydes: Ring opening reactions of epoxydes.

UNIT III: CHEMISTRY OF BENZENE AND ITS DERIVATIVES**15 hrs.**

Aromaticity – criteria for aromaticity – aromatic and non-aromatic cyclic – polycyclic and heterocyclic compounds – aromaticity and annulenes – chemical consequences of aromaticity – antiaromaticity – molecular orbital description of aromaticity and non-aromaticity – non-benzenoid aromatic compounds.

Benzene – nomenclature – structure of benzene – Kekule structure – reactions of benzene – arenes – reactions of alkyl benzenes – reduction – oxidation – substitution in ring and side chain – alkenyl benzene – reactions of alkenyl benzenes – substitution – addition – polymerization

Aryl Halides : Nucleophilic aromatic substitution – unimolecular – bimolecular displacement (S_NAr) mechanism – elimination – addition (benzyne) mechanism – alkyl halides Vs aryl halides.

UNIT IV: AROMATIC ELECTROPHILIC SUBSTITUTION**15 hrs.**

General mechanism for electrophilic substitution – arenium ions – mechanism – halogenations – nitration – Friedel-Crafts alkylation – limitation – Friedel-Crafts acylation – Friedel-Crafts alkylation vs Friedel-Crafts acylation – sulphonation – orientation and reactivity in mono substituted and disubstituted benzene – introduction – effect of substituents – orientation – relative reactivity – classification of substituents – orientation in disubstituted benzenes – reactivity and orientation – theory of reactivity and orientation – electron release via resonance – effect of halogen on electrophilic substitution.

UNIT V: POLYNUCLEAR HYDROCARBONS**15 hrs.**

Introduction – naphthalene – nomenclature – isomerism – structure – chemical properties – electrophilic aromatic substitution reactions – orientation of disubstitution – addition reactions – oxidation – derivatives of naphthalene – naphthols, naphthylamines – naphthoic acids – naphthaquinones – anthracene – nomenclature – isomerism – structure – chemical properties – reduction – oxidation – electrophilic substitution reactions – formylation – electrophilic addition – dimerization – Diels-Alder reaction – phenanthrene – nomenclature – isomerism – structure – chemical properties – addition – oxidation – ozonolysis – reduction – sulphonation – nitration.

TEXT BOOK(S)

Jain. M. K. and Sharma, S. C., (2013). *Modern Organic Chemistry*, (4th ed.), New Delhi: Vishal Publishing. Print

Morrison R. T and Boyd R.N., (2008). *Organic Chemistry*, (7th ed.), New Delhi: Prentice Hall. Print

REFERENCE BOOK(S)

Mehta, B. & Mehta, M., (2005). *Organic Chemistry*, (1st ed.), New Delhi, PHI Learning Pvt. Ltd. Print
Paula Yurkanis Bruice, (2002). *Organic Chemistry*, (3rd ed.), New Delhi, Pearson education, Inc., Print
Solomons T.W.G., (2004). *Organic Chemistry*, (8th ed.), Singapore, John Willey & Sons Inc., Print
Wade L.G. & Singh. M.S., (2006). *Organic Chemistry*, (6th ed.), Delhi, Pearson education, Inc.,
Print

CHE3505CM THERMODYNAMICS AND CHEMICAL EQUILIBRIA (THEORY)

LEARNING OUTCOMES:

On successful completion of the course, the student will be able to

- relate the laws of thermodynamics to different thermodynamic processes
- explain the energetics of chemical systems using the concepts of thermodynamics
- evaluate the significance of various thermodynamic parameters
- analyze the equilibrium conditions for various types of chemical reactions
- explain the behavior of acids, bases and salts in solutions

COURSE CONTENT:

5 hrs./wk.

UNIT I: FIRST LAW OF THERMODYNAMICS AND THERMOCHEMISTRY

15 hrs.

Importance and limitations of thermodynamics – terms and definitions: systems – boundary – surroundings – macroscopic properties – homogeneous and heterogeneous systems – thermodynamic equilibrium – intensive and extensive properties – state variables – thermodynamic processes – nature of work and heat – first law – internal energy and first law – state and path functions – exact and inexact differentials – enthalpy – heat capacity – expansion of an ideal gas – reversible and irreversible – work done in isothermal and adiabatic expansions – comparison of isothermal and adiabatic expansions – Joule-Thomson effect – Joule-Thomson coefficient in ideal gas – zeroth Law of thermodynamics Thermochemistry: exothermic and endothermic reactions – thermochemical equations – enthalpy of a reaction – variation of enthalpy of reaction with temperature – different types of enthalpy of reaction – Hess's law and applications – bond energy – measurement of heat of reaction.

UNIT II: SECOND LAW OF THERMODYNAMICS

15 hrs.

Limitations of the first law – spontaneous processes and criteria of spontaneity – cyclic processes – Carnot cycle – heat engine – efficiency – Carnot theorem – other forms of second law – concept of entropy from Carnot cycle – entropy changes: isothermal expansion – reversible and irreversible processes – phase change – mixture of ideal gases – standard entropy – physical significance of entropy – work and free energy functions – variation of free energy with temperature and pressure – Maxwell relations – criteria for reversible and irreversible processes – Gibbs-Helmholtz equation.

UNIT III: THERMODYNAMICS OF OPEN SYSTEMS AND THIRD LAW

15 hrs.

Partial molar properties – chemical potential – Gibbs-Duhem equation – Clausius-Clapeyron equation – differential and integrated forms – applications of the equation – concept of fugacity and activity – third law of thermodynamics – Nernst heat theorem – determination of absolute entropies of solids– liquids and gases – absolute entropies of elements and compounds – experimental verification of third law – limitations to the third law – entropy changes in chemical reactions – residual entropy.

UNIT IV: CHEMICAL EQUILIBRIUM**15 hrs.**

Reversible reactions – nature and characteristics of chemical equilibrium – law of mass action – thermodynamic derivation of law of chemical equilibrium – Van't Hoff reaction isotherm – equilibrium constant – equilibrium constant expression in terms of partial pressures – relationship between K_p and K_c – calculations involving K_p – units of equilibrium constant – temperature dependence of equilibrium constant – homogeneous and heterogeneous equilibria – Van't Hoff equation – Le-Chatelier's principle.

UNIT V: IONIC EQUILIBRIUM**15 hrs.**

Acid and base theories – Arrhenius concept – Lowry-Brønsted concept – Lewis concept – dissociation of a weak acids and bases – dissociation constants of polybasic acids – dissociation of a weak base – ionic product of water – pH scale – common ion effect – buffer solutions – buffer mixtures of a weak acid/ weak base and its salt – Henderson's equation – hydrolysis of salts – hydrolysis constant – relation between K_h , K_a and K_w – degree of hydrolysis – pH of hydrolysed salt solutions – salts of weak acids and strong bases – strong acids and weak bases – weak acids and weak bases – degree of hydrolysis– pH of their salt solutions – determination of degree of hydrolysis – acid-base indicators – theories of indicators – pH titration – solubility product and its applications.

TEXT BOOK(S):

Arun Bahl, B.S. Bahl and G.D. Tuli, (2014). *Essentials of Physical Chemistry*, (revised ed.), India: S. Chand and company private limited. Print.

Puri, B.R., Sharma L.R. and M. S. Pathania. (2019). *Principles of Physical Chemistry*, (48th ed.), Jalandhar: Vishal Publishing Co. Print.

REFERENCE BOOK(S):

Julio de Paula and Peter Atkins, (2016). *Atkin's Physical Chemistry*, (10th ed.), New Delhi: Oxford University Press. Print.

**CHE3506CM CHEMISTRY OF s- AND p- BLOCK ELEMENTS
(THEORY)****5 hrs./wk.****LEARNING OUTCOMES:**

On successful completion of the course, the student will be able to

- classify acids and bases and balance redox reactions
- illustrate the properties of hydrogen and hydrides
- explain the importance of the compounds of s- block and p-block elements
- discuss the structure and bonding in compounds
- identify the role of inorganic compounds in day today life

COURSE CONTENT:**UNIT I: REDOX REACTION****15 hrs.**

Oxidation number and oxidation state – rules for calculating oxidation number – oxidation and reduction – redox and half reactions – oxidizing and reducing agents – autooxidation – induced oxidation – balancing redox equations by oxidation number and ion-electron methods.

Acids and bases: Concept of acids and bases – Arrhenius concept – Lowry-Brønsted concept – Lux-Flood concept – Cady-Elsey concept – Lewis concept – Usanovich – HSAB principle – strength of hydracids.

UNIT II: HYDROGEN AND s- BLOCK ELEMENTS

15 hrs.

Position of hydrogen in the periodic table – resemblance of hydrogen with alkali metals and with halogens – nascent hydrogen – ortho and para hydrogen – isotopes of hydrogen – heavy water – hydrides – classification of hydrides: ionic – molecular – interstitial hydrides – applications of hydrogen and hydrides in fuel cells.

General characteristics and periodicity in the properties of group I and II elements – diagonal relationship of lithium and magnesium – beryllium and aluminium – comparison of lithium and beryllium with their respective group members – complexes of alkali and alkaline earth metals.

UNIT III: BORON AND CARBON GROUP

15 hrs.

Compounds of boron and aluminium – comparative study: hydrides – oxides – halides – structure and bonding in Boranes: (B_2H_6 , B_4H_{10}) – boron nitride – borazine – preparation, properties, structure and uses: Boric acid and borax – Lithium aluminium hydride.

Anomalous behaviour of carbon – comparison of carbon and silicon – allotropy of carbon – diamond – graphite – fullerene – graphene – intercalation compounds of graphite – structure of oxides – oxyacids and their salts – carbides and their classification – properties and uses of silica – classification and structure of silicates – preparation and properties of stannous chloride – white and red lead.

UNIT IV: NITROGEN AND OXYGEN GROUP

15 hrs.

Compounds of nitrogen group elements – hydrides – halides – oxohalides – oxides of nitrogen – (N_2O_3 , N_2O_5 , NO_2 , N_2O) – oxoacids of nitrogen (HNO_2 , HNO_3) – oxoacids of phosphorus (H_3PO_2 , H_3PO_3 , $H_4P_2O_6$, H_3PO_4) – structure of hydrazine – hydrazoic acid – urotropine – phosphazine – liquid NH_3 . Anomalous behaviour of oxygen – oxides and their classification – ozone – preparation and properties – hydrogen peroxide – structure and properties of oxides (SO_2 , SO_3) and oxoacids of Sulphur – (H_2SO_4 , H_2SO_5 , $H_2S_2O_8$) – structure of oxo halides of Sulphur ($SOCl_2$, SO_2Cl_2).

UNIT V: HALOGENS AND NOBLE GASES

15 hrs.

Anomalous behaviour of fluorine – compounds of halogens – hydrogen halides – oxides – oxoacids – structure of interhalogen compounds: ICl , ClF_3 , IF_5 , IF_7 – poly halides (ICl_4^-) – pseudohalogens: cyanogen – pseudohalides – comparison of halogens and pseudo halogens – liquid HF . Properties and uses of noble gases – compounds of noble gases : hydrates – clathrates – structure of xenon compounds: fluoride (XeF_2 , XeF_4 , XeF_6) – oxy fluorides ($XeOF_2$, $XeOF_4$, XeO_2F_2 , XeO_2F_4 , XeO_3F_2) – oxides (XeO_3 , XeO_4) – compounds of krypton and radon.

TEXT BOOK (S):

Gurdeep Raj, (2015). *Advanced Inorganic Chemistry*, (35th ed.), Meerut: Krishna Prakashan Media Private limited. Print.

B. R. Puri, L. R. Sharma and K. C. Kalia, (2017). *Principles of Inorganic Chemistry*, (31st ed.), Delhi: Vishal Publishing Co. Print.

REFERENCE BOOK (S):

R. D. Madan, (2016). *Modern Inorganic Chemistry*, (3rd ed.), New Delhi: S. Chand and Company Private limited. Print.

CHE3201CP EXPERIMENTAL ORGANIC CHEMISTRY I

(LAB)

3 hrs./wk.

LEARNING OUTCOMES:

On successful completion of the course, the student will be able to

- estimate the organic compounds using titrimetry
- apply the principles of green chemistry in the preparation of organic compounds
- develop a suitable method for the synthesis of industrially important compounds
- analyze the phytochemical components present in the natural products

COURSE CONTENT:

45 hrs.

I. ORGANIC ESTIMATION

15 hrs.

- a. Estimation of phenol/aniline
- b. Estimation of Glucose –Lane and Enyon method
- c. Estimation of ketone

II. GREEN SYNTHESIS: Solid state and Microwave assisted

25 hrs.

- a. Synthesis of Diazonium Dyes
- b. Synthesis of Chalcone
- c. Aldol condensation/Benzoin Condensation
- d. Benzilic acid rearrangement
- e. Synthesis of any one heterocyclic compound

III. Extraction of Natural product (any one)

5 hrs.

REFERENCE BOOK(S):

Brian S. Furniss, Antony J Hannaford, Peter W. G. Smith & Austin R. Tatchell, (1989). *Vogel's Textbook of Organic Chemistry*, (5th ed.), London: ELBS. Print

Donald L Pavia, Gary M.Lampman & George S Kritz, (2009). *Organic Chemistry – A Lab Manual*, , New Delhi: Sengage Learning. Print

Gnanapragasam N.S, Ramamurthy G, (2013). *Organic Chemistry Lab Manual*, Chennai: S.Viswanathan (Printers and Publishers) PVT.LTD. Print

CHE3202CP EXPERIMENTAL INORGANIC CHEMISTRY

(LAB)

3 hrs./wk.

LEARNING OUTCOMES:

On successful completion of the course, the student will be able to

- classify anions and cations
- apply green principles for qualitative analysis of salt mixture
- explain the chemical principles involved in the analysis of salt mixtures
- identify the environmentally sensitive ions present in water and soil samples
- relate the toxicity of metal ions to health

COURSE CONTENT:

Qualitative analysis of salt mixture – analysis of a salt mixture containing two acid radicals and two basic radicals – with one interfering acid radicals – discussion on heavy metal toxicity.

Acid radicals

CO_3^{2-} , NO_3^- , CH_3COO^- , Cl^- , Br^- , I^- , SO_4^{2-} , PO_4^{3-} , BO_3^{3-} , F^- , $\text{C}_2\text{O}_4^{2-}$, CrO_4^{2-} , $\text{S}_2\text{O}_3^{2-}$, $\text{C}_4\text{H}_4\text{O}_6^{2-}$.

Basic radicals

Pb^{2+} , Bi^{3+} , Cu^{2+} , Cd^{2+} , Sb^{3+} , Fe^{3+} , Al^{3+} , Cr^{3+} , Co^{2+} , Ni^{2+} , Zn^{2+} , Mn^{2+} , Ba^{2+} , Sr^{2+} , Ca^{2+} , Mg^{2+} , NH_4^+ , K^+ .

REFERENCE BOOK(S):

Mala Nath, (2016). *Inorganic Chemistry: A Laboratory Manual*, New Delhi: Narosa Publishing House Pvt. Ltd. Print.

Ramanujam, V. V. (2012). *Inorganic Semi Micro Qualitative Analysis*, (3rd ed.), Chennai: The National Publishing Company. Print.

Svehla, G. (1996). *Vogel's Qualitative Inorganic Analysis*, (7th ed.) India: Pearson. Print.

CHE4504CM STEREOCHEMISTRY AND CARBONYL COMPOUNDS

(THEORY)

LEARNING OUTCOME:

5 hrs./wk.

On successful completion of the course, the student will be able to

- identify the stereoisomerism exhibited in the organic compounds
- examine the various conformations of cyclohexane derivatives
- illustrate the condensation reactions of aldehydes and ketones
- assess the chemistry of aliphatic and aromatic carboxylic acids and its derivatives
- compare the acidic properties of carboxylic acids and substituted carboxylic acids

COURSE CONTENT:

UNIT I: STEREOISOMERISM I

15 hrs.

Chirality – chiral centre – enantiomers – R and S – sequence rules – Fischer Projection – Sawhorse & Newmann representations of 2,3-dibromobutane, 2,3-dihydroxybutane, 2-bromo-3-hydroxybutane – inter conversions – configuration – Diastereomers – odd and even chiral centers

– meso structure – resolution – racemic modification – substitution at chiral carbon – optical activity due to chiral axis – optical activity of allenes and spiranes – atropisomerism of biphenyls – chiral plane – cyclophanes and ansa compounds – molecular overcrowding – asymmetric synthesis.

E / Z notation for double bonded compounds ($\text{C} = \text{C}$) – physical and chemical methods used in distinguishing geometrical isomers.

UNIT II: STEREOISOMERISM II

15 hrs.

Definition of conformation – configurational and conformational isomers – conformational isomerism in ethane – n-butane – 1,2-dibromoethane – ethylene glycol with energy profile diagrams – stability of conformers – Baeyer's strain theory – stereoisomerism of cyclohexane – monosubstituted cyclohexanes.

UNIT III: ALIPHATIC AND AROMATIC CARBONYL COMPOUNDS

15 hrs.

Structure and reactivity of carbonyl group – nucleophilic addition reactions – reaction with carbon nucleophiles – oxygen nucleophiles – nitrogen nucleophiles – sulphur nucleophile – oxidation reactions of aldehydes and ketones – distinguishing aldehydes from ketones – reduction reactions of carbonyl compounds – Catalytic reduction – reduction with metal hydrides – MPV reduction – Wolff – Kishner reduction – Clemmenson's reduction.

UNIT IV: REACTIONS OF ALDEHYDES AND KETONES

15 hrs.

Acidity of a hydrogen – keto-enol tautomerism – acid catalysed halogenation – aldol condensation – dehydration of aldol products – crossed aldol condensation – reactions related to the aldol condensation with mechanism – claisen condensation – crossed Claisen condensation – Benzoin condensation – Claisen – Schmidt – Cannizzaro's reaction – Crossed Cannizzaro reaction – Mannich reaction – Reactions of α , β -unsaturated compounds – Michael addition (recall) – Perkin – Knoevenagel – Stobbe condensations.

UNIT V: CARBOXYLIC ACIDS AND THEIR DERIVATIVES

15 hrs.

Preparation – physical properties and reactions of monocarboxylic acids: comparison of acidity of various carboxylic acids – preparation and reactions of acid chlorides – anhydrides – esters and amides comparative study of nucleophilic substitution at acyl group – Mechanism of acidic and alkaline hydrolysis of esters – Dieckmann and Reformatsky reactions – Hofmann – bromamide degradation and Curtius rearrangement – Sulphonic acid – acidity of substituted acids – typical reactions of dicarboxylic acids : succinic acid – phthalic acid – ketoacids: pyruvic acid – acetoacetic acid – hydroxy acids: lactic – malic – tartaric – citric – salicylic acid – unsaturated acids: maleic – fumaric – cinnamic acid.

TEXTBOOK(S):

Jain, M. K. Sharma, S. C; (2013). *Modern Organic Chemistry*, (4th ed.), New Delhi: Vishal Publishing Co. Print. UNITS (I, III & V).

Paula Yurkanis Bruice, (2002). *Organic Chemistry*, (3rd ed.), Delhi: Pearson education, Inc, Print. (UNITS II & IV).

REFERENCE BOOK(S)

Bhupinder Mehta, Manju Mehta, (2005). *Organic Chemistry*, (1st ed.), Delhi: PHI Learning Pvt. Ltd. Print.

Morrison, R. T., Boyd R. N., (2008). *Organic Chemistry*, (7th ed.), New Delhi: Prentice Hall. Print.

Solomons T. W. G., (2004). *Organic Chemistry*, (8th ed.), Singapore: John Willey & Sons Inc. Print.

CHE4505CM BEHAVIOUR OF GASES AND LIQUIDS

(THEORY)

LEARNING OUTCOME:

5 hrs./wk.

On successful completion of the course, the student will be able to

- apply the gaseous laws to understand the behaviour of gases
- analyse the causes of deviation of real gases from ideal behaviour
- determine the properties of liquids through suitable experiments
- analyse the behavior of solutions

- classify the various types of colloids used in day-to-day life

COURSE CONTENT:

UNIT I: IDEAL GASES

15 hrs.

General characteristics of gases – parameters of a gas – gas laws – Boyle's law – Charles's law – combined gas law – Gay Lussac's law – Avogadro's law – Ideal gas equation – Dalton's law of partial pressures – kinetic molecular theory of gases – derivation of kinetic gas equation – distribution of molecular velocities – different kinds of velocities – calculation of molecular velocities – collision parameters.

UNIT II: REAL GASES

15 hrs.

Deviations from ideal behavior – compressibility factor – effect of temperature – explanation for deviations – equation of state of real gases – van der Waals' equation – other equations of state limitations – critical phenomena – critical constants – critical temperature from P-V isotherms – continuity of state – van der Waals equation and critical constants – critical compressibility factor – law of corresponding states – experimental determination of critical constants – methods of liquefaction of gases.

UNIT III: LIQUIDS

15 hrs.

Intermolecular forces of attraction (Recall) – Vapour pressure – effect of temperature on vapour pressure – methods of determination of vapour pressure – effect of vapour pressure on boiling point – surface tension – effect of temperature on surface tension – methods of determination of surface tension – Viscosity – measurement of viscosity – effect of temperature on viscosity – refractive index – specific and molar refraction – determination of refractive index – molar refraction and chemical constitution – optical activity – specific rotation – measurement of optical activity.

UNIT IV: SOLUTIONS

15 hrs.

Solutions of liquids in liquids – Ideal solutions – Raoult's law – vapour pressures of ideal solutions – activity of a component in an ideal solution – Gibbs-Duhem-Margules equation – thermodynamics of ideal solutions – Real solutions – types of non-ideal solutions – completely miscible binary solutions and types – fractional distillation of binary liquids of different types – lever rule – distillation of immiscible liquids – partially miscible liquids – types – phenol-water system – aniline-hexane system – triethylamine-water system – nicotine-water system.

Solutions of gases in liquids – factors influencing solubility of a gas – Henry's law – comparison of Henry's law and Raoult's law. The Distribution law – thermodynamic derivation – association of solute in one of the solvents – dissociation of solute in one of the solvents – solute entering into chemical combination with one of the solvents – applications of distribution law – solvent extraction.

UNIT V: COLLIGATIVE PROPERTIES AND COLLOIDS

15 hrs.

Colligative Properties – lowering of vapour pressure – elevation in boiling point – depression in freezing point – osmotic pressure – determination of molecular weight – van't Hoff factor.

Colloids – types of colloids – lyophilic and lyophobic sols and their characteristics – preparation – dispersion – aggregation – purification – dialysis – optical properties – kinetic properties – electrical

properties of colloids – gold number – stability of sols – associated colloids – cleansing action of soaps and detergents – emulsions – gels – applications of colloids.

TEXTBOOK(S):

Arun Bahl, Bahl B.S. and Tuli G.D., (2009). *Essentials of Physical Chemistry*, New Delhi: S. Chand and Co. Ltd. Print. (Unit III & V).

Puri B.R, Sharma L.R and Pathania S., (2012). *Principles of Physical Chemistry*, (46th ed.), New Delhi: Vishal Publishing Co. Print. (Unit I – II & IV).

REFERENCE BOOK:

Atkins P.W., (2006). *Physical Chemistry*, (8th ed.), New York: Oxford University Press. Print.

CHE4404CM CHEMISTRY OF TRANSITION ELEMENTS

(THEORY)

LEARNING OUTCOME:

4 hrs./Wk.

On successful completion of the course the student will be able to

- recognise the importance of inorganic polymers
- identify the characteristics of d and f - block elements
- discuss the chemistry of transition elements
- compare the properties of Lanthanides and Actinides

COURSE CONTENT:

UNIT I: GENERAL CHARACTERISTICS OF d-BLOCK ELEMENTS

12 hrs.

General properties – size – density – melting point – boiling point – reactivity of metals – ionisation potentials – colour – magnetic properties – paramagnetism – diamagnetism – ferromagnetism – antiferromagnetism – catalytic properties – variable valency – stability of various oxidation states – ability to form complexes – non-stoichiometry – Position of elements of the transition series in the periodic table.

UNIT II: FIRST TRANSITION SERIES

12 hrs.

Preparation – properties and uses – titanium compounds – titanium dioxide – titanium tetrachloride – chromium compounds – chromic oxide – chrome alum – potassium chromate – potassium dichromate – chrome red – chromyl chloride. Iron compounds – ferrous sulphate – Mohr's salt – potassium ferrocyanide and ferricyanide – Prussian blue and Turnbull's blue – rusting of iron – nickel compounds – nickel sulphate – nickel dimethyl glyoximate – Copper compounds – copper sulphate – verdigris – alloys of copper.

UNIT III: SECOND AND THIRD TRANSITION SERIES

12 hrs.

Preparation – properties and uses – molybdenum compounds – molybdenum blue – ammonium molybdate – tungsten compounds – tungstic acid – tungsten bronze – platinum compounds – chloroplatinic acid – complexes of platinum – mercury compounds – mercurous chloride – mercuric chloride – mercuric sulphide – mercuric iodide – Millon's base – Nessler's reagent – amalgams.

UNIT IV: LANTHANIDES AND ACTINIDES

12 hrs.

General discussion – occurrence – isolation – separation techniques – oxidation states – lanthanide contraction – colour – magnetic and spectral properties – actinides – general properties – comparison of lanthanides and actinides.

UNIT V: INORGANIC POLYMERS

12 hrs.

General properties – classification – phosphorus-based polymers – chain polymer – network polymer – phosphate glasses – crystalline polymetaphosphates – sulphur based polymers – polymeric sulphur nitrides – chalcogenides glasses – Boron based polymers – polycarboranes – polymeric boron nitrides – silicon-based polymers – organosilicons – preparation – structures – applications.

TEXTBOOK(S):

Puri B.R., Sharma L.R., Kalia K.C., (2010). *Principles of Inorganic Chemistry*, (31st ed.), Delhi: Milestone Publishers and Distributors. Print.

REFERENCE BOOK(S)

Atkins P., Overton T., Rourke J., Weller M., Armstrong. F. Shriver & Atkins., *Inorganic Chemistry* (4th ed.), New Delhi: Oxford University Press. Print.

Lee J.D., A (2002) *New Concise Inorganic Chemistry*, (5th ed.) London: ELBS. Print.

CHE4405CM INTRODUCTION TO CHEMINFORMATICS

(THEORY)

LEARNING OUTCOME:

4 hrs./Wk.

On successful completion of the course the student will be able to

- recognise the different types of 2D and 3D molecular representations
- identify the database models
- describe the applications of various databases
- analyse the activity of the drug molecules
- evaluate the druglikeliness of molecules

COURSE CONTENT:

UNIT I: CHEMICAL REPRESENTATION OF MOLECULES

12 hrs.

History and evolution of cheminformatics – use of cheminformatics – prospects of cheminformatics – representation of chemical compounds – line Notations – WLN – ROSDAL – SMILES – SMARTS – SYBYL – InCHI – basics of graph theory – matrix representations – adjacency – distance – atom – connectivity and bond matrix – connection table – various file formats – structure of molfiles – sfiles and PDB – library and toolkits – special notations of chemical structures – markush structures – fragment coding – fingerprints – hashed fingerprints – hash codes – representation of 3D structures – z-matrix – representation of chemical reactions – different electronic effects : reaction classification.

UNIT II: DATABASES AND CHEMICAL STRUCTURE SEARCHING

12 hrs.

Molecular structure searching techniques – full structure – super structure – substructure and similarity searching methods – similarity based on 2D fingerprints – Tanimoto and Tversky – dice coefficient – cosine – Euclidean distance – properties of similarity and distance coefficient. Databases sources – contents– design – accessibility and use – chemical database – PUBCHEM–

CHEMBANK – DRUGBANK – JCHEM – CAS Registry – ZINC – MOLTABLE – literature database – PUBMED – biological database – chemPDB – KEGG – GenBank– NCI.

UNIT III: MOLECULAR DESCRIPTORS AND STRUCTURE-ACTIVITY RELATIONSHIP **12 hrs.**

Introduction – classification – descriptors calculated from 2D structure – simple counts – physicochemical properties – molar refractivity – topological indices – kappa shape indices – 2D fingerprints – descriptors based on 3D representations – pharmacophore keys – quantitative structure – activity relationships(QSAR) – graphs and equations– physicochemical properties– hydrophobicity – electronic effects – steric effects – Hansch equation – craig plot – topliss scheme– bioisosteres – free wilson approach – planning a QSAR study – Case study – 3D QSAR – case studies: design of thymidylate synthase inhibitor – design of serotonin antagonist as a possible anxiolytic agent.

UNIT IV: INTRODUCTION TO DRUG-DESIGN AND DISCOVERY **12 hrs.**

Drug-discovery – historical perspective – identification and validation of therapeutic targets – enzymes – receptors – proteins – nucleic acids – lipids – carbohydrates – drug development process – discovery of drug candidates – natural products – lead development and optimization – rule of five – prediction of ADME properties – role of molecular recognition in drug design – thermodynamic consideration of drug binding – H-bonding – salt bridge interactions – stereochemistry in drug design.

UNIT V: DOCKING **12 hrs.**

Docking procedures – rigid docking – flexible docking and scoring functions: structure based de novo design techniques – molecular docking – active site characterization – case study of designing HIV I protease inhibitor – quantitative structure – property relationships (QSPR) – predicting melting point – solubility – boiling point – TPSA – quantitative structure toxicity relationships (QSTR) – aquatic toxicity – carcinogenicity – mutagenicity.

TEXTBOOK(S):

Patrick, G.L., (2009). *An introduction to medicinal chemistry*, (4th ed.), United kingdom: Oxford university press, Print.

Larsen P.K. (ed), Stromgaard. K(ed), Madsen. U (ed), (2004). *Textbook of Drug Design and Discovery*, (4th ed.), London and New York: Taylor and Francis Group. Print.

REFERENCE BOOK(S)

Leach, A.R., Gillet V.J, (2007). *An Introduction to Chemoinformatics*, (revised ed.), Netherland: Springer. Print.

Kar, A., (2006). *Medicinal Chemistry*, New Delhi: New Age International publisher. Print. Ganellin C.R., Roberts S.M., (1993). *Medicinal chemistry, the role of organic chemistry in drug research*, (2nd ed.), Elsevier. Print.

Gasteiger, J. (ed.), Engel, T (ed.), (2003). *Chemoinformatics: A Textbook*, Weinheim: Wiley VCH. Print.

Leach A.R., (2001). *Molecular Modelling: Principles and applications*, (2nd ed.), New Delhi: Prentice Hall. Print.

Patrick G. L., (2002). *Instant notes Medicinal chemistry*, Viva books private limited. Print.

CHE 4202CP EXPERIMENTAL ORGANIC CHEMISTRY II

(LAB)

LEARNING OUTCOME:

3 hrs. / wk.

On successful completion of the course, the student will be able to

- find the elements other than carbon, hydrogen and oxygen present in the compound
- classify the nature of the organic compound
- analyse the functional groups present in the organic compound
- justify the presence of the functional group by preparing a suitable derivative

COURSE CONTENT:

QUALITATIVE ANALYSIS OF THE FOLLOWING ORGANIC COMPOUNDS

45 hrs.

Phenol

Aldehydes

Ketones

Carboxylic acids

Esters

Nitro compounds

Amine

Amide

Diamide

Carbohydrates (mono- and di- saccharides)

REFERENCE BOOK(S):

Gnanaprasadam N. S., Ramamurthy G., (2013). *Organic Chemistry Lab Manual*, Chennai: S. Viswanathan (Printers and Publishers) Pvt. Ltd. Print.

CHE4203CP EXPERIMENTAL PHYSICAL CHEMISTRY I

(LAB)

LEARNING OUTCOME:

3 hrs./wk.

On successful completion of the course, the student will be able to:

- apply the principles of electro chemistry, kinetics and phase equilibria to carry out the experiments
- make use of the instruments to acquire data
- analyse and represent the data in a suitable form
- design experiments based on the concepts

COURSE CONTENT:

45 hrs.

CONCEPT & EXPERIMENT

Viscosity of liquids

Determination of viscosity of solvents using Ostwald's Viscometer

Optical activity

Determination of specific rotation of sugar solution by Polarimeter
Miscibility of liquids
Critical solution temperature of partially miscible liquid system
Effect of electrolytes on CST
Partition coefficient
Partition coefficient for the distribution of Iodine between water and CCl₄
Buffers
Preparation of buffer mixtures and determination of pH of various Buffer mixtures
Acid–base indicators
Determination of working range of indicators
pH–Acidity vs. alkalinity
pH titration of a strong acid with a base
Self–designed experiment by the student based on any one of the above concepts.

TEXTBOOK(S):

Viswanathan B. and Raghavan P.S., (2017). *Practical Physical Chemistry*, New Delhi: Viva Books Pvt. Ltd. Print.

CHE4203SP CHEMINFORMATICS LAB

(Lab)

LEARNING OUTCOME:

2 hrs./wk.

On successful completion of the course, the student will be able to

- build molecules and optimize its geometry
- convert the molecules into various file formats
- interpret the HOMO/LUMO of the molecule
- analyse the toxicity of drug molecules

COURSE CONTENT:

EXPERIMENTS / LAB EXERCISES: 30 hrs.

Construction of molecules in Argus Lab, MarvinSketch and ChemSketch [6 hrs.]

Retrieving the SMILES notation of the molecules [2 hrs.]

Converting the molecules into different file [2 hrs.]

Calculation of isoelectric point of amino acids [2 hrs.]

Determination of solubility of drug molecules [2 hrs.]

Determination of log P [2 hrs.]

Energy Optimization [4 hrs.]

Determination of HOMO/LUMO band gap energy in benzene [2 hrs.]

Retrieving toxicological data from web sources for QSAR, QSPR and QSTR related studies [4 hrs.]

Docking a lead compound into the active site of the target [4 hrs.]

REFERENCE BOOK(S):

Andrew R, Leach, Valerie J. Gillet, (2007). *An Introduction to Chemoinformatics*, (revised ed.),

Netherland: Springer. Print.

Johann Gasteiger(ed.), Thomas Engel (ed.), (2003). *Cheminformatics: A Textbook*, Weinheim: Wiley VCH. Print.

Leach A.R, (2001). *Molecular Modelling: Principles and applications*, (2nd ed.), New Delhi: Prentice Hall. Print.

**CHE5504CM CHEMISTRY OF NITROGEN COMPOUNDS AND REARRANGEMENTS
(THEORY)**

5 hrs./wk.

LEARNING OUTCOMES:

On successful completion of the course, the student will be able to

- summarize the reactions of amines and nitro compounds
- examine the structure, synthesis and reactions of nitrogen containing biomolecules
- illustrate the synthesis and reactivity of heterocyclic compounds
- outline the mechanistic details of rearrangements exhibited in organic compounds
- relate the structure of the dyes and pigments to their properties

COURSE CONTENT :

UNIT I : AMINES AND NITRO COMPOUNDS

15 hrs.

Amines: Nomenclature – structure of amines – physical properties – preparation – Gabriel phthalimide synthesis – basicity – effect of substituent and solvent on the basicity of aliphatic and aromatic amines – basicity and steric effects – Libermann nitroso test – Schotten-Baumann reaction – carbylamine reaction – distinction between 1^o, 2^o and 3^o amines – Hofmann's method – Hinsberg reagent and nitrous acid – conversion of amines into substituted amides.

Diazonium Salts: Preparation – coupling reactions – synthetic applications of diazonium salts.

Nitrocompounds: Preparation and reactions of nitroalkanes – Nef reaction and Mannich reaction leading to Michael addition and reduction – tautomerism of nitroalkanes – distinction between nitroalkanes and alkylnitrites.

UNIT II: NUCLEIC ACIDS, AMINOACIDS AND PROTEINS

15 hrs.

Components of nucleic acids – nucleosides and nucleotides – ATP – role as energy carrier – kinetic stability of ATP in cell – ATP coupled reactions – structure, synthesis and reactions of: Adenine – Guanine – Cytosine – Uracil and Thymine – structure of polynucleotides – amino acids – peptides and their classification – α -amino acids – synthesis – ionic properties and reactions – Zwitterions – pKa values – isoelectric point and electrophoresis – study of peptides: determination of their primary structures – end group analysis – methods of peptide synthesis – synthesis of peptides using N-protecting – C-protecting and C-activating groups – solid-phase synthesis.

UNIT III: HETEROCYCLIC COMPOUNDS

15 hrs.

Introduction – nomenclature – five membered rings: preparation & structure of furan – pyrrole Thiophene – electrophilic substitution – reactivity and orientation – derivatives – Knorr-pyrrole synthesis – Paal-Knorr synthesis – indole – preparation – Fischer-Indole synthesis – properties Six membered rings: Pyridine – synthesis – structure – basicity of pyridine – electrophilic substitution – nucleophilic substitution – Chichibabin reaction.

UNIT IV : REARRANGEMENTS

15 hrs.

Types of molecular rearrangements – rearrangement involving migration of a group or atom – pinacol-pinacolone rearrangement – Wagner-Meerwein – Benzil-benzilic acid rearrangement – rearrangement to electron deficient nitrogen: Beckmann – Schmidt – Hofmann – Lossen and Curtius rearrangement – rearrangement involving migration of a group from oxygen to aromatic ring – Fries and Claisen rearrangement – rearrangement to electron – deficient oxygen: Baeyer-Villiger oxidation – hydroperoxide rearrangement – Dakin reaction – Hofmann-Martius rearrangement – Fischer-Hepp rearrangement – Diazoamino – aminoazo rearrangement – Benzidine rearrangement.

UNIT V: DYES and PIGMENTS

15 hrs.

Theories of colour and chemical constitution – dyes-classification – chemistry of dyes – triphenyl amine dyes – nitro and nitroso dyes – azo dyes – phthalein and xanthene dyes – anthraquinone dyes – indigoid dyes – fluorescent brightening agents – pigments-anthocyanins – flavones – phthalocyanines – carotenoids – chlorophyll – food colours – certified colorants – natural non-toxic pigments – spurious colours.

TEXT BOOK(S):

Jain M. K. and Sharma, S. C., (2013). *Modern Organic Chemistry*, (4th ed.), New Delhi: Vishal Publishing, Print. (Unit I & IV).

Morrison R. T. and Boyd R.N., (2008). *Organic Chemistry*, (7th ed.), New Delhi: Prentice Hall, Print. (UNITS II, III & V).

REFERENCE BOOK(S):

Agarwal O. P. (2007). *Chemistry of natural products* (32nd ed. / Vol. II), Meerut: Goel Publishing House. Print

Chatwal Gurdeep, (2008). *Chemistry of natural products* (5th ed./ Vol. II). Delhi: Himalaya publishing House. Print

Finar I. L. (2011). *Organic Chemistry* (Vol. I & II, 8th ed.) Pearson Education. Print

Paula Yurkanis Bruice, (2002). *Organic Chemistry*, (3rd ed.), Delhi, Pearson education, Inc. Print

Solomons T.W.G., (2004). *Organic Chemistry*, (8th ed.), Singapore, John Willey & Sons Inc. Print

Wade L.G. and Singh. M.S., (2006). *Organic Chemistry*, (6th ed.), Delhi, Pearson education, Inc. Print.

CHE5505CM CHEMICAL KINETICS, CATALYSIS AND ELECTROCHEMISTRY (THEORY)

5 hrs./wk.

LEARNING OUTCOMES:

On successful completion of the course, the student will be able to

- describe the kinetics of chemical reactions
- describe the mechanism and applications of adsorption
- demonstrate the importance of catalysts in chemical and biological reactions
- explain the types of conductance and applications
- examine the efficiency of electrochemical cells based on electrochemical and thermodynamic parameters

COURSE CONTENT:

UNIT I: CHEMICAL KINETICS I**15 hrs.**

Introduction – rate of reaction – rate equation – rate constant – order of reaction – unit of rate constant – integration of rate expressions – first – second – third – zero order reactions – half-life time of first – second – n^{th} order reactions – methods of determining the order of a reaction – order and molecularity of simple and complex reactions – mechanism of a complex reaction – the equilibrium approximation – the steady – state approximation.

UNIT II: CHEMICAL KINETICS II AND SURFACE CHEMISTRY**15 hrs.**

Theories of reaction rates – collision theory of bimolecular gaseous reactions – effect of temperature on reaction rates – activation energy – effect of catalyst – activated complex theory of bimolecular reactions – Lindemann theory of unimolecular gaseous reactions and limitations – Surface Chemistry: Adsorption vs. absorption – types of adsorption – physisorption and chemisorption – adsorption of gases by solids – factors affecting adsorption – Freundlich and Langmuir isotherms – different types of adsorption isotherms – applications of adsorption.

UNIT III: CHEMICAL CATALYSIS**15 hrs.**

General characteristics of catalytic reactions – catalysis – negative catalysis – promoters – catalytic poisons – autocatalysis – types of catalysis – homogeneous catalysis – acid-base catalysis – enzyme catalysis – effect of temperature on enzyme catalysis – Michaelis-Menten equation – heterogeneous catalysis – Langmuir-Hinshelwood mechanism – kinetics of surface reactions – unimolecular and bimolecular surface reactions – pH dependence of catalyzed reactions.

UNIT IV: ELECTROCHEMISTRY I**15 hrs.**

Faraday's law of electrolysis – Ohm's law – conductance – specific conductance – equivalent conductance – molar conductance – determination of electrical conductance – cell constant – variation of molar conductance with dilution – ionic mobility – Hittorf's theoretical device – transport number – determination of transport number – Hittorf's and moving boundary method – Kohlrausch's law and its applications – diffusion and ionic mobility – applications of conductance measurements – Ostwald's dilution law – Debye-Hückel theory of strong electrolytes – Debye-Falkenhagen and Wien effects – Onsager's equation (no derivation) – mean ionic activity coefficient – ionic strength.

UNIT V: ELECTROCHEMISTRY II**15 hrs.**

Galvanic cells – Daniel cell – reversible electrodes: metal-metal ion – gas electrode – metal-insoluble metal salt – oxidation –reduction electrodes – single electrode potential – standard electrode potentials – electrochemical series – electromotive force of galvanic cell – representation of a cell – determination of standard emf of a cell – effect of concentration on electrode potential – Nernst equation – relation between emf and thermodynamic parameters – emf and equilibrium constant – concentration cells – electrode-concentration cells – electrolyte-concentration cells – liquid junction potential – application of emf measurements – determination of pH of a solution – potentiometric titrations.

TEXT BOOK(S):

Arun Bahl, B.S. Bahl and G.D. Tuli, (2014). *Essentials of Physical Chemistry*, (revised ed.), India: S. Chand and company private limited. Print.

Puri, B.R., Sharma L.R. and M. S. Pathania. (2019). *Principles of Physical Chemistry*, (48th ed.), Jalandhar: Vishal Publishing Co. Print.

REFERENCE BOOK(S):

Peter Atkins and Julio de Paula, (2016). *Atkin's Physical Chemistry*, (10th ed.), New Delhi: Oxford University Press. Print.

**CHE5506CM COORDINATION AND BIOINORGANIC CHEMISTRY
(THEORY)**

5 hrs./Wk.

LEARNING OUTCOMES:

On successful completion of the course, the student will be able to

- classify the ligands and name the coordination compounds
- apply bonding theories in determining the electronic and magnetic properties of coordination compounds
- relate the role of metals to the toxicity in biological systems
- illustrate the structural aspects of carbonyls and nitrosyls
- identify the different types of crystal structure and analyze the change in properties due to crystal defects

COURSE CONTENT:

UNIT I: CO-ORDINATION CHEMISTRY I

15 hrs.

Introduction – Werner's theory – types of ligands – nomenclature – isomerism – types – stability of complexes – bonding in complexes – Valence bond theory: inner and outer orbital complexes – Crystal field theory: Octahedral – tetrahedral – square planar complexes – high spin and low spin complexes – CFSE: Factors affecting crystal field splitting – Jahn –Teller effect – nephelauxetic effect – MOT: octahedral complexes – tetrahedral – square planar complexes – spectrochemical series – comparison of VBT, CFT & MOT.

UNIT II: CO-ORDINATION CHEMISTRY II

15 hrs.

Spectral and magnetic properties of metal complexes: term symbols – electronic spectra of complexes (d^1 and d^9) – electronic absorption spectrum of $[\text{Ti}(\text{H}_2\text{O})_6]^{3+}$ ion – elementary treatment of Orgel diagrams – types of magnetic behavior – spin-only formula – calculation of magnetic moments.

Reactivity of metal complexes – labile and inert complexes – ligand substitution reactions – S_N1 , S_N2 and S_N1CB substitution reactions of square planar complexes – trans effect.

UNIT III: BIO - INORGANIC CHEMISTRY

15 hrs.

Role of alkali and alkaline earth metals in biological systems – Na^+/K^+ pump – structure of heme – role of hemoglobin and myoglobin in biological systems – structure of chlorophyll – biological functions and toxicity of metals: Cr, Mn, Fe, Co, Cu, Mo, Zn – nitrogen fixation.

UNIT IV: CARBONYLS AND NITROSYLS

15 hrs.

Carbonyls – classification – general methods of preparation – properties – structure and bonding – mononuclear carbonyls: $\text{Cr}(\text{CO})_6$, $\text{Fe}(\text{CO})_5$, $\text{Ni}(\text{CO})_4$ – binuclear carbonyls: $\text{Mn}_2(\text{CO})_{10}$, $\text{Co}_2(\text{CO})_8$, $\text{Fe}_2(\text{CO})_9$, $\text{Fe}_3(\text{CO})_{12}$ – EAN and 18 electron rule as applied to carbonyls.

Nitrosyls – types – nitrosyl compounds – preparation – properties – structure – sodium nitroprusside – nitroferrous sulphate – EAN and 18 electron rule as applied to nitrosyls.

UNIT V: SOLID STATE CHEMISTRY**15 hrs.**

Types of solids – isotropy and anisotropy – symmetry of crystals – Miller indices – crystal structure – cubic unit cells – X-ray crystallography – Bragg's equation – methods of determination of diffraction angle – classification of crystals on the basis of bonds – ionic crystals (NaCl, CsCl) – molecular crystals – network covalent crystals – metallic crystals – structure of metallic crystals – close packing – limiting radius ratio – crystal defects – Schotky and Frenkel defects.

TEXT BOOK(S):

James E. Huheey, Ellen A. Keiter, Richard L. Keiter and Okhil K. Medhi, (2013). *Inorganic Chemistry*, (4th ed.), New Delhi: Pearson Education. Print. (Units I, II, III)

Lee J. D., (2002). *A New Concise Inorganic Chemistry*, (5th ed.), London: ELBS. Print. (Unit II)

Puri B. R, Sharma L. R and Kalia.K. C., (2013). *Principles of Inorganic Chemistry*, (31st ed.) New Delhi: Vallabha publications. Print. (Units IV & V)

REFERENCE BOOK(S):

Azaroff L., (2000). *Introduction to Solids*, (19th reprint), New Delhi: Tata McGraw Hill Publishing Company. Print.

Madan R. D. (2016). *Modern Inorganic Chemistry*, (3rd ed.), New Delhi: S. Chand and Company Private limited. Print.

Malik U., Madan R. D and Tuli G. D. (2007). *Selected Topics in Inorganic Chemistry*, New Delhi: S. Chand and company. Print.

Mark Weller, Tina Overton, Jonathan Rourke and Fraser Armstrong. (2016). *Inorganic Chemistry*, (6th ed.) New Delhi: Oxford University Press. Print.

CHE5203CP EXPERIMENTAL PHYSICAL CHEMISTRY II**(LAB)****LEARNING OUTCOMES:**

On successful completion of the course, the student will be able to

- apply the principles of electro chemistry, kinetics and phase equilibria to carry out the experiments
- make use of the instruments and collect data
- analyze interpret and represent the experimental data.
- design an experiment based on the concepts

COURSE CONTENT:**3 Hrs./Wk.****EXPERIMENTS / LAB:****45 hrs.****Theoretical concepts of the experiments****6 hrs.****Electrochemical conductance****15 hrs.**

1. Determination of cell constant, specific conductance and molar conductance of a strong electrolyte
2. Determination of dissociation constant of a weak electrolyte (acetic acid)
3. Determination of solubility, solubility product of sparingly soluble salts
4. Conductometric titration of strong /weak acid vs weak/strong base

Beer-Lambert's law**3 hrs.**

5. Determination of ϵ_{\max} and concentration of potassium permanganate solution

Electromotive force	3 hrs.
6. Determination of standard reduction potential and cell emf	
Chemical kinetics	6 hrs.
7. Determination of rate constant of acid catalyzed hydrolysis of ester	
Phase Diagram	6 hrs.
8. Construction of Phase Diagram of a simple system	
One self-designed experiment by the student based on any one of the following concepts:	
Electrochemical conductance/ Beer-Lambert's law/ Electromotive force/ Chemical kinetics/ Phase Diagram	6 hrs.

REFERENCE BOOK(S):

Ahluwalia V.K., Sumitha Dingra and Adarsh Gulati, (2005). *College Practical Chemistry*, Hyderabad, India: University Press Pvt Ltd. Print

Gary D. Christian, (2011). *Analytical Chemistry*, (6th ed.), Kundli: John Wiley & Sons, Print

Peter Mathews G, (1985) *Experimental Physical Chemistry*, Oxford:Clarendon Press, Print

Raghavan, P. S., Viswanathan B., (2017). *Practical Physical Chemistry*, NewDelhi: Viva books Private limited. Print

**CHE5201CM INTRODUCTION TO RESEARCH METHODOLOGY
(THEORY)**

LEARNING OUTCOME : **2 Hrs./wk.**

On successful completion of the course, the student will be able to

- Recognize the purpose of research.
- Classify the methods of research.
- Apply the knowledge of e-resources in literature search.
- Write a scientific report based on the research done.

COURSE OUTLINE :

UNIT-I : INTRODUCTION AND CHOICE OF THE PROBLEM **7 Hrs.**

Introduction to research process -scientific methods- characteristics of scientific method - formulation of hypothesis – classification of research – fundamental, applied and action – selection of problem - preparing a proposal - research design - methods of research – experimental, historical, case study and survey.

UNIT-II : LITERATURE SEARCH **8 Hrs.**

Introduction to chemical abstracts – subject index, substance index, author index, and formula index and other indices- uses of these indices with examples, methods of using the titles and index – importance of impact factor of journals – impact factor analysis - use of e-resources for literature search and downloading – basics of internet services –various sources of abstracts, articles and papers of browsing and downloading, techniques of conversion from one format to another.

UNIT-III : DATA ANALYSIS **8 Hrs.**

Statistical analysis of data, mean, median and mode, (recall) mean deviation and standard deviation, gaussian distribution, comparison of results – student's *t*-test, *f* test, propagation of error-rejection of data, linear least square fit, correlation coefficient.

UNIT-IV : PRESENTATION OF REPORT

7 Hrs.

Ethics of research - plagiarism - planning the introduction - body of the report, footnotes and endnotes – page and chapter format – margin - indentation – placement of tables and figures and numbering of tables and figures - writing bibliography -books, journals and websites - concepts of patents and patenting

TEXT BOOK(S)

Dawson, catherine, *practical research methods*, new delhi: ubs, publishers distributors, 2002.print.

Gary d. Christian, *analytical chemistry*, 6th edition: john wiley & sons, 2003. Print.

Gurumani n., *scientific thesis writing and paper presentation*, chennai: mjp publishers, 2010.print.

John w. Best, *research and education*, 3rd edition, new delhi: prentice hall of india private ltd, 1978. Print.

Kumar, ranjit, *research methodology-a step-by-step guide for beginners*, 2nd edition, singapore: pearson education, 2005. Print.

CHE0602LM FOOD ANALYSIS (THEORY)

LEARNING OUTCOMES:

On successful completion of the course, the student will be able to

- identify the nutrients present in food
- examine the presence of food additives and common food adulterants in food and food products
- elaborate the adverse effects of pesticide residues in food
- apply the various analytical techniques to analyze the chemical contamination in food and food products
- inspect the foodborne illnesses and create awareness to the community

COURSE CONTENT:

4 hrs./Wk.

SECTION I:

15 hrs.

COMMON UNIT

Understanding Life Frontier Engagement

- a. Service-Learning and Life Frontier Engagement
- b. Principles – engagement, reflection, reciprocity, public dissemination
- c. Meaning of community and understanding of community dynamics
- d. Programme planning in Life Frontier Engagement – stages: Need analysis, Problem identification, Goal setting, Concept finalization, planning for stages of research, research and analysis, reflection and dissemination of results.
- e. Ethical concerns in Life Frontier Engagement – Confidentiality, Conflict of interest, Informed consent.

ACTIVITY MODULE FOR SECTION I:

- a) (i) Facilitate students to understand the concept of Service-Learning and Life Frontier Engagement based on the information in the reading material given using student centered learning activities.
- ii) Interaction with a local community (Example: Children, adolescents, adults within or outside college) to identify community dynamics.
- (iii) Need based analysis to be done on the community by framing a questionnaire for base line socio-economic survey.
- b) (i) Students to prepare a programme plan based on the sub-themes and target group identified by the department.
- (ii) Presentation by teams by refining the ideas of students based on program planning stages.
- c) Activity based on case studies relevant to ethical issues in community engagement.

CONCEPT SECTION II: THEMATIC CONCEPTS

15 hrs.

Site Assessment and Planning: A Conceptual Approach Classification concept:

- Classification of food products based on the nutritional values
- List of food additives (preservatives, nutritional additives, coloring agents, flavoring agents, emulsifiers and stabilizers, artificial sweetener) in processed food
- List of adulterants in various food products
- Types of pesticide residues in food

Correlation concept:

- If the amount of food additives exceeds the acceptable daily intake (ADI), it may lead to harmful health effects
- Long-term consumption of pesticide contaminated food product leads to acute and chronic health effects
- Malnutrition results in diet-related noncommunicable diseases

Theoretical concept:

- Food plays a major role for the well-being of a person. The health of a person gets affected
- by excess intake of processed food which contains additives
- while consuming food with pesticide residue
- by consuming adulterated food
- Effective remedial measures through healthy dietary plan can help the person to overcome malnutrition and the ill-effects of harmful chemicals

ACTIVITY MODULE FOR SECTION II:

- Identification of the various food additives present in processed food
- Quick tests for common food adulterants: milk and milk products, oils and fats, sugars and confectionaries, food grains and its products, spices and condiments
- Analysis of various nutrients present in food products
- Detection of presence of pesticides residues in food
- Sensitization of the community through awareness programme

SECTION III: COMMUNITY ENGAGEMENT PROCESS

15 hrs.

- A community which needs to be sensitized about the food related issues will be identified
- Survey will be carried out in the selected community

- Detection/determination of additives, adulterants and pesticide residues in food samples and comparison with the standard values (permissible limit) will be carried out
- The data will be analyzed, based on the results effective remedial measures will be suggested to the community

The student will document her engagement with the community through this process in the form of a report with supporting evidences (geo-tagged photographs, video, community feedback etc.).

The student will present her outcome of learning process in the form of an oral presentation.

REFERENCE BOOK(S):

Begum, R. (2008). *A Textbook of Food, Nutrition and Dietetics*, (3rd revised ed.), New Delhi:

Sterling publishers Pvt. Ltd. Print

Branen, A. L., Davidson, P. M., Salminen, S. and Thorngate III, J. H. (2002) *Food Additives*, (2nd

Ed. Revised and Expanded), New York: Basel, Marcel Dekker, Inc. Print

Meyer, L. H. (1987) *Food Chemistry*, Delhi: CBS Publishers & distributors. Print

Mudambi & Rao, (2006) *Food Science*, New Delhi: Wiley Eastern limited. Print

CHE6505CM ORGANIC SYNTHESIS AND SPECTROSCOPY

(Theory)

LEARNING OUTCOME:

5 Hrs./Wk.

On successful completion of the course, the student will be able to

- identify the basic principles of organic synthesis
- recognize the importance of green synthesis
- Illustrate the role of synthetically important compounds in organic synthesis.
- realize the usage of spectral studies in structural determination

COURSE OUTLINE:

UNIT I: ORGANIC SYNTHESIS:

15 Hrs.

Importance of Organic synthesis – steps involved in synthetic planning (one illustration each) – carbon-carbon bond formation (Michael addition, aldol condensation, Wittig reaction, enolate alkylation, Diels Alder reaction) – functional group interconversion (from carbonyl, nitro, amino to other functional groups) – Introduction to disconnection approach (Terms and definitions) – protecting groups (Carbonyl and diol protection).

UNIT II: SYNTHETICALLY IMPORTANT COMPOUNDS AND REAGENTS

15 Hrs.

Active methylene compounds – Preparation and synthetic uses of diazomethane, malonic ester, acetoacetic ester, diazoacetic ester, cyanoacetic ester.

Organometallic compounds of Mg, Li and Cu – synthetic applications

UNIT III: GREEN SYNTHESIS

15 Hrs.

Introduction to green chemistry – principles of green synthesis – green catalysts (Zeolites, montmorillonite, clay) – green solvents – water, supercritical CO₂, ionic liquids (imidazolium salts) – solvent less reactions – phase transfer catalysts – types of biocatalyst in organic synthesis – microwave assisted green synthesis – ultra sound assisted synthesis.

UNIT IV: ORGANIC SPECTROSCOPY I

15 Hrs.

Electronic spectroscopy – Electronic transitions – designation of various transitions – Chromophores, Auxochromes – bathochromic, hypsochromic, hyperchromic and hypochromic shifts – solvent effects – Woodward rules for calculation of λ_{max} for dienes, polyenes and carbonyl compounds.

Mass Spectrometry – Mass spectrum – determination of molecular weight, molecular formulae – isotopic abundance – molecular ion – metastable ions – fragmentation routes – fragmentations associated with hydrocarbons – hydroxyl compounds, ethers, ketones, aldehydes, acids, halogen compounds with one Cl / Br atoms (both aliphatic and aromatic compounds to be done simultaneously). Concept for virtual lab

Effect of conjugation, HOMO and LUMO of molecules

UNIT V: ORGANIC SPECTROSCOPY II

15 Hrs.

IR spectroscopy – Skeletal vibrations of organic molecules – factors influencing vibrational frequency of bonds – hydrogen bonding, electronic effect, mass effect, conjugation, ring size – identification of functional groups using IR data. NMR – Nuclear spin states and NMR active nuclei – nuclear magnetic moments – mechanism of resonance absorption – population of nuclear spin states, proton NMR – interaction of spin magnetic moment of a proton with external magnetic moment, chemical shift and shielding, chemical equivalence, chemical environment and chemical shift, magnetic anisotropy, spin-spin splitting – proton NMR spectra of organic molecules – applications – structural elucidation of organic molecules using proton NMR spectral data – introduction to ^{13}C NMR – ^{13}C chemical shifts – proton decoupled ^{13}C spectra.

Concept for virtual lab

Molecular vibrations-IR

TEXT BOOK(S):

Mohan, Jag. (2004). *Organic spectroscopy: principles and applications* (2nd ed.). New Delhi: Narosa Publishing House. Print.

Jain, M. K., and Sharma, S. C. (2005). *Modern organic chemistry* (4th ed.). New Delhi: Vishal Publication Co. Print.

REFERENCE BOOK(S):

Mackie, R. K., and Smith, D. M. (1982). *Guidebook to Organic Synthesis*. England: ELBS. Print. Pavia, Chapman and Kriz, (2007). *Introduction to Spectroscopy* (3rd ed.). Asia: Thomson. Print. Robert E. Ireland, (1969). *Organic Synthesis*. India: Prentice-Hall of India Pvt. Ltd. Print. Silverstein, Bassler and Morrill, (1991). *Spectrometric Identification of Organic Compounds* (5th ed.). New York: John Wiley and Sons. Print.

Stuart Warren, (2004). *Organic Synthesis. The Disconnection Approach*. New York: John Wiley & Sons. Print.

William Kemp, (1991). *Organic Spectroscopy* (4th ed.). England: ELBS. Print.

WEBSITE(S):

<http://www.chemtube3d.com/spectrouv-CE.html><http://www.chemtube3d.com/spectrovibcd1-CE-final.html>

CHE6506CM MOLECULAR SPECTROSCOPY, QUANTUM CHEMISTRY AND GROUP THEORY

(THEORY)

LEARNING OUTCOME:

5 hrs./wk.

On successful completion of the course, the student will be able to

- distinguish different types of spectroscopic techniques
- apply the principles of spectroscopy to molecules
- describe the behavior of quantum mechanical systems
- predict the symmetry of elements and point groups of molecules

COURSE CONTENT:

UNIT I: PHYSICAL PRINCIPLES OF MOLECULAR SPECTROSCOPY I

15 hrs.

Introduction to EMR – regions of EMR and types of spectroscopy – basic features of spectrometers – signal to noise ratio – resolving power – line width and Intensity of spectral lines – Microwave spectroscopy – classification of rotators – rotational spectra of rigid and non-rigid diatomic molecules – determination of bond length – Isotopic mass – dipole moment of molecules – Infra-Red Spectroscopy – vibrations in a molecule – energy of a diatomic molecule – vibrational spectrum of simple harmonic and anharmonic oscillators – fundamentals – overtones and hot bands – fundamental vibrations and symmetry in polyatomic molecules.

UNIT II: PHYSICAL PRINCIPLES OF MOLECULAR SPECTROSCOPY II

15 hrs.

Raman Spectroscopy – Rayleigh and Raman scattering – classical and quantum theories – rotation – Raman and rotation – Vibration Raman spectrum of a diatomic molecule – Rule of Mutual Exclusion. Electronic Spectroscopy – Born-Oppenheimer approximation – Franck Condon Principle – Dissociation and Predissociation. Electron spin resonance – Principle of resonance absorption – ESR spectrum of an unpaired electron – Hyperfine structure – ESR spectra of Hydrogen atom and methyl radical.

UNIT III: QUANTUM MECHANICS I

15 hrs.

Wave – particle duality of light and matter – de Broglie equation – Heisenberg uncertainty principle – Planck's quantum theory – black body radiation – photoelectric effect – operators in quantum mechanics – Hermitian operators – commuting and non-commuting operators – eigen functions and eigenvalues – Schrodinger wave equation – particle in 1D and 3D box.

UNIT IV: QUANTUM MECHANICS II

15 hrs.

Wave functions – characteristics – wave function and probability – normalisation of wave function – postulates of quantum mechanics – wave functions of particle in 1D and 3D box – quantization of energy – allowed energies and degeneracy of energy levels – orthogonality – orthonormal wave functions – Hamiltonian for the hydrogen and helium atoms. Introduction to statistical thermodynamics – micro and macro states – ensembles – probability distribution using Maxwell-Boltzmann – Bose-Einstein – Fermi-Dirac statistics (no derivation).

UNIT V: GROUP THEORY

15 hrs.

Symmetry and geometry (recall VSEPR theory) – Symmetry elements and symmetry operations – products of symmetry operations – symmetry point groups – Schoenflies notations – properties of a group – group multiplication tables – sub groups – classes – similarity transformations – representation of a group matrix representation of symmetry operations – reducible and irreducible representations – properties of the characters of representation – Great Orthogonality theorem – construction of character tables – C_{2v} and C_{2h} point groups.

TEXTBOOK(S):

Banwell. N & Mc Cash. M., (1994). *Fundamentals of Molecular Spectroscopy*, New Delhi: Tata McGraw Hill Publishing Co Ltd. Print. (Units I & II)

Donald A Mc Quarrie, (2011). *Quantum Chemistry*, India: Viva Books Pvt. Ltd. Print. (Units III & IV).

Salahuddin Kunju A. & Krishnan G., (2015). *Group theory and its applications in Chemistry*, (2nd ed.) Delhi: PHI Learning Pvt. Ltd. Print. (Unit V)

REFERENCE BOOK(S):

Ramakrishnan V. & Gopinathan M.S., (1998). *Group Theory In Chemistry*, Vishal Publications, Print.

Swarnalakshmi S., Saroja T., Ezhilarasi R. M., (2008). *A simple approach to group theory in chemistry*, Hyderabad: University Press. Print.

CHE6507CM CHEMISTRY OF NATURAL PRODUCTS**(THEORY)****LEARNING OUTCOME:****5 hrs./wk.**

On successful completion of the course, the student will be able to

- examine the structure and functions of carbohydrates
- analyse the structure and properties of alkaloids and terpenoids
- summarize the significance of steroids and hormones
- recognise the structure and properties of lipids
- explain the structure and importance of vitamins

COURSE CONTENT:**UNIT I: CARBOHYDRATES****15 hrs.**

Monosaccharides – classification – family tree of saccharides – configuration of aldoses in relation to glyceraldehyde – constitution of glucose and fructose – stereochemistry of glucose – oxidation – interconversions – lower aldose to higher aldose – Kiliani synthesis – Ruff degradation – conversion of an aldose into its epimer – aldose into ketose – mutarotation of glucose – configuration of glucose – absolute configuration – cyclic structure of D+) glucose – configuration about anomeric carbon – methylation – determination of ring size – conformations of glucose – disaccharides – General study of cellobiose – sucrose – (structure and specific properties) Haworth structure.

UNIT II: ALKALOIDS AND TERPENOIDS**15 hrs.**

Alkaloids – definition – extraction – general properties – general methods of determining structure classification – structural elucidation and synthesis of pyridine and piperidine group – piperine pyridine and pyrrolidine group – Cocaine.

Terpenoids – Introduction – classification – isolation – isoprene rule and special isoprene rule– general methods of determining the structure – structure and synthesis of acyclic terpenoid – citral bicyclic terpenoid– camphor.

UNIT III: STEROIDS AND HORMONES**15 hrs.**

Classification and biological importance of steroids – Diels' hydrocarbon – cholesterol – occurrence properties – test and physiological activity – structure of steroid hormones – progesterone –

androsterone – adrenocortical hormones – bile acids – phytosterols – non steroid hormones – structure and functions of thyroid gland hormones – adrenal gland hormones.

UNIT IV: LIPIDS

15 hrs.

Biological functions – classification – natural fats – difference between fats and oil – fats – nomenclature – physical and chemical properties – rancidity – analysis of fats and oils – acid value – saponification value – iodine value – Reichert – Meissl value – distinction between animal and vegetable fats – uses – compound lipids – phospholipids : lecithins – cephalins – plasmalogens – phosphoinositides – phosphosphingosides – glycolipids.

UNIT V: VITAMINS

15 hrs.

Classification – vitamin A and vision – structure – function and deficiency diseases – vitamin D, E, K, B1, B3, Bc, B6, niacin and B12 – structural elucidation and synthesis of vitamin A, B2 and K.

TEXTBOOK(S):

Jain, M. K. and Sharma, S. C., (2013). *Modern Organic Chemistry*, (4th ed.), New Delhi: Vishal Publishing. Print.

Morrison, R.T, Boyd, R. N. and Bhattacharjee S. K., (2011). *Organic Chemistry*, (7th ed.), New Delhi: Pearson. Print.

REFERENCE BOOK(S):

Agarwal, O. P; (2007). *Chemistry of natural products, Vol. II*, (32nd ed.), Meerut: Goel Publishing House. Print

Chatwal Gurdeep, (2008). *Chemistry of natural products , Vol. II*, (5th ed.), Delhi: Himalaya publishing House. Print.

Finar I. L., (2011). *Organic Chemistry, Vol. I & II*, (8th ed.), Delhi: Pearson Education. Print.

CHE6502CT PHOTOCHEMISTRY, PHASE EQUILIBRIA AND INSTRUMENTAL ANALYSIS

(LAB CUM THEORY)

LEARNING OUTCOME:

4T + 2L hrs./wk.

On successful completion of the course the student will be able to

- apply the principles of photochemistry in chemical and biochemical reactions
- identify the various phases components and degrees of freedom to describe a system
- classify polymers that are used in daily life
- apply the theoretical knowledge to handle analytical instruments for various applications

COURSE CONTENT:

UNIT I: PHOTOCHEMISTRY

15 hrs.

Principles of photochemistry – consequences of light absorption – Jablonski diagram – light absorption by solutions – laws of photochemistry – quantum yield and its determination – primary and secondary processes – photochemical reactions – photochemical rate law – kinetics of photochemical reactions – formation of hydrogen chloride and hydrogen bromide – photophysical processes – chemiluminescence – bioluminescence – photosensitization – quenching – applications of photochemistry – laser action.

UNIT II: PHASE EQUILIBRIA**15 hrs.**

Difference between phase and state of matter – definition of terms – phase – components and degrees of freedom – derivation of Gibb's phase rule – phase diagrams of one component systems – water – sulfur – liquid Helium – two component systems – simple eutectic systems – thermal analysis and cooling curves – phase diagrams of Pb-Ag and KI – water systems – freezing mixtures – formation of compounds with congruent and incongruent melting points – Ferric chloride-water – sodium sulphate-water systems.

UNIT III: POLYMER CHEMISTRY**15 hrs.**

Introduction – classification of polymers – degree of polymerization – polydispersity and polydispersity index – molar mass of polymers – number average and mass average molar mass – determination of molar mass of polymers – osmometry and viscometry – types of polymerization – kinetics of addition and condensation polymerization – industrially important polymers – preparation and applications of Nylon 66 – Nylon 6 – Dacron – bakelite – melamine – neoprene – buna-N – buna-S – Teflon – biopolymers and its applications.

UNIT IV: ELECTRIC AND MAGNETIC PROPERTIES**15 hrs.**

Electric properties of molecules – polarization in an electric field – Clausius – Mosotti equation – Debye equation – symmetry and dipole moment – measurement of dipole moment – dependence of polarisability on frequency – bond moments – group moments – dipole moments and molecular structure. Magnetic properties of molecules – magnetic permeability – magnetic susceptibility – para and dia magnetism – molecular interpretation of para and dia magnetism – measurement of magnetic susceptibility – ferro and antiferromagnetism.

UNIT V: INSTRUMENTAL METHODS OF ANALYSIS**30 hrs.**

Principles and method of analysis using Atomic Absorption Spectroscopy – Fluorimetry – Thermo Gravimetry – Differential Thermal Analysis – Amperometry – Coulometry – Voltammetry. The students will be trained in the following instruments with respect to the principle– working and applications.

Flame photometer – Determination of Na and K in different samples Nephelometer – Determination of sulphate ion in different samples TDS analyser – Determination of total dissolved salts in water samples

UV-Visible Spectrophotometer – Determination of λ_{max} of coloured samples UV-Photoreactor – Photocatalytic degradation of natural and synthetic dye samples

TEXTBOOK(S):

Madan R.D., (2011). *Modern Inorganic Chemistry*, (3rd ed.), New Delhi: S. Chand & Co. Ltd. Print.

Arun Bahl, Bahl B.S. and Tuli G.D., (2009). *Essentials of Physical Chemistry*, New Delhi: S. Chand and Co. Ltd. Print.

Gowariker, Viswanathan and Jayadev Sreedhar, (1986). *Polymer Science*, New Delhi: Wiley Eastern Ltd. Print.

Puri B.R, Sharma L.R and Pathania S., (2012). *Principles of Physical Chemistry*, (46th ed.), New Delhi: Vishal Publishing Co. Print.

Skoog D.A., West D.M., Holler F.J., Crouch S.R., (2014). *Fundamentals of Analytical Chemistry*, India: Cengage Learning. Print.
