DEPARTMENT OF CHEMISTRY

B.Sc. (Special) - Chemistry with Cheminformatics
Course Content - 2013 Batch

CHE1101FS 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
- comprehend 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-conjunctionpunctuation marks- articles- paragraph- construction of paragraph- linkage and cohesion-summary-Precise –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)

S.R.Inthira and V. Saraswathi, **Enrich Your English Book I: Communication Skills**, Oxford New York, Oxford University Press, 1995.

Essentials of Language – Instructor Manual, **Skilledge an initiative of ICT Academy of Tamil Nadu**, 2011.

WEBSITE(S) :

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

http://eltvoices.in/Volume1/Issue1/EVI11.5.pdf

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

http://www.sharadavikas.com/CourceMeterials/btc34.PDF

CHE 1201FM PRINCIPLES OF BIOMOLECULES

THEORY

LEARNING OUTCOMES: **3 hrs / week**

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

- acquire knowledge about the cell structure
- identify the structure and dynamics of biomolecules.
- relate the biomolecules with their specific functions.
- illustrate the role of biomolecules in different metabolic pathways

UNIT I CELL STRUCTURE **11hrs**

Introduction-prokaryotic and eukaryotic cells-development of multicellular organisms. Cell structure-Organelles – Cell environment, cell-cell interactions. Transport of biomolecules.

UNIT II STRUCTURE OF BIOMOLECULES **11 hrs**

A structural study on the assembly of amino acids to proteins, nucleotides to nucleic acids, monosaccharides to linear and branched polysaccharides, phospholipids to biomembranes. (covalent and non-covalent interactions) – Structural transformation of biomolecules in solutions.

UNIT III FUNCTIONS OF BIOMOLECULES **11 hrs**

Functions of biomolecules-Carbohydrates- energy storage and cell recognition process, Lipids – energy storage, as components of cell membrane and cell signaling, Nucleic acids – carriers of coded information, Proteins – as structural and functional proteins.

UNIT IV MAJOR METABOLIC PATHWAYS **12hrs**

Bioenergetics –Energy producing and energy utilizing systems. Thermodynamic relationships and energy rich compounds - Reactions and importance of major metabolic pathways - catabolic pathways: β- oxidation of lipids, Glycolysis - Tricarboxylic acid cycle, urea cycle - anabolic pathway: Lipogenesis, glycogenesis.

REFERENCE BOOKS:

Geoffrey. M. Cooper., Robert E. Hausman, **The Cell, A Molecular Approach**, 5th edition, ASM press. Sinauer Associates Corporation. USA. 2009. (Unit I, II)

Lodish, Berk, Kaiser.et.al., **Molecular Cell Biology**, 6th edition, W. H. Freeman and Company, New York.2008 (Unit II, III)

Thomas M. Devlin, **Textbook of biochemistry with clinical correlations**, 7th edition, John Wiley & Sons, Inc., USA.2011 (Unit IV)

CHE 1301FM BASICS OF CHEMISTRY

THEORY

LEARNING OUTCOMES: **4 hrs/week**

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

- review the evolution of Chemistry
- apply the IUPAC rules to name organic compounds
- predict the configuration of stereoisomers
- analyze and interpret the gradation in the properties of elements in the periodic table
- inspect all types of redox reactions
- employ a proper laboratory technique to perform experiments

COURSE OUTLINE:

UNIT I HISTORY OF CHEMISTRY- **12hrs**

From fire to atomism – Origin of metallurgy and alchemy – alchemy to chemistry – Early chemists - (300 BCE-300 CE)- Robert Boyle and the origins of modern chemistry - Antoine Lavoisier and the revolution in chemistry – Theory of vitalism and Wohler's synthesis - Isolation and structure of benzene- Evolution of Periodic Table – Quantum Chemistry – origin of Biochemistry – Chemical industries – An overview on the historical development of organic, inorganic and physical chemistry - Nobel laureates in chemistry - Women in chemistry.

Unit II A.NOMENCLATURE OF ORGANIC COMPOUNDS **6hrs**

IUPAC nomenclature -rules for naming organic compounds-alkanes, alkenes, alkynes, cyclic 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.

II B. BASICS OF STEREOCHEMISTRY 6hrs

Stereoisomerism – enantiomerism – plane polarized light and specific rotation – optical activity – Properties of enantiomers – racemic modification and resolution – assignment of configuration – R and S – sequence rule – diastereomers – meso structure – Geometric isomerism of alkenes.

UNIT III PERIODIC TABLE AND ATOMIC PROPERTIES 12hrs

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 IV REDOX REACTIONS 12hrs

Covalency, Oxidation number and oxidation state – Rules for calculating oxidation number - oxidation – reduction reactions – oxidizing and reducing agents- Auto and induced oxidation– Balancing redox reactions by oxidation number method and ion electron method – Electrochemical redox reactions – electrode potential – standard electrode potentials – The electrochemical series - electromotive force of Galvanic cells and feasibility of electrochemical cell reactions based on electrochemical series – balancing the electrochemical redox reactions.

UNIT V BASICS OF LABORATORY TECHNIQUES 12hrs

Lab safety measures - Handling of glassware – Purification of organic compounds - Preparation of solutions- different concentration units – normality, molarity, molality, mole fraction, ppm, mole percent and mass percent. Primary and secondary standard –Equivalent weight of acids, bases, oxidizing and reducing agents, Saturated, unsaturated and supersaturated solutions. Electrolytes and non electrolytes.

REFERENCE BOOK(S):

Datta N.C., **The story of Chemistry**, First Edition, University's Press Pvt Ltd., India, 2005, (UNIT I)

Thomas N. Sorrell, **Organic Chemistry**, First Edition, Viva Books Pvt Ltd., India, 2004 (UNIT I)

Bhupinder Mehta , Manju Mehta, **Organic Chemistry,** First edition**,** PHI Learning Pvt. Ltd., 2005. (UNIT IIa)

Morrison R.T., Boyd R.N. and Bhattacharjee S.K., **Organic Chemistry**, Seventh edition, Pearson Education, India, 2011 (UNIT IIb)

Gary D. Christian, **Analytical Chemistry**, Sixth edition, John Wiley & Sons, 2011 (UNITV)

Madan R.D., **Modern Inorganic Chemistry**,Third edition, S. Chand & Company Ltd., 2011. (UNIT III & UNIT IV)

Puri.B.R, Sharma.L.R and Pathania.S., **Principles of Physical Chemistry** , 50th edition , Shoban Lal Nagin Chand & Co., New Delhi, 2011. (UNIT IV)

CHE 1401CM GENERAL CHEMISTRY

THEORY

LEARNING OUTCOMES: **5 hrs/week**

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

- correlate the structure and behaviour of atom
- differentiate the various chemical interactions in molecules through bonding concepts
- explain the nuclear reactions and their importance
- predict the nuclear transmutations
- identify the role of radioactive materials in different applications
- appraise the role of chemistry in various fields

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 –Wave-particle duality of matter - de Broglie's equation-Heisenberg's uncertainity principle.

UNIT II CHEMICAL BONDING –LEWIS CONCEPT **15hrs**

Chemical bond -types of bonds – ionic bond –factors favoring the formation and 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 of ionic and covalent 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 III CHEMICAL BONDING – ORBITAL CONCEPT 15hrs

Linnett's DQ theory - VSEPR theory – VBT of covalent bond – formation of sigma and pi bonds – Resonance structures of CO, CO_2, CO_3^{2-}, O_3, SO_2,SO_3 - hybridisation – sp-sp^2-sp^3 – sp^3d – sp^3d^2 hybridisation – Molecular orbital theory – LCAO method – bonding and antibonding orbitals – formation of MOs in homonuclear and heteronuclear diatomic molecules and ions.

UNIT IV NUCLEAR CHEMISTRY AND RADIOACTIVITY 15hrs

NUCLEAR CHEMISTRY

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.

UNIT V: HUMAN TOUCH OF CHEMISTRY 15hrs

Applications of chemistry in daily life – food, clothes, fuels, plastics, paints and varnishes, dyes, medicine, therapeutic drugs, cosmetics, fertilizers, insecticides, explosives, building materials

Applications in different fields – Forensic science – Food processing - Energy conservation and storage-electronics-**Interesting scientific queries in day-today life and simple solutions through chemistry** – **Societal and Ethical issues of chemistry.**

REFERENCE BOOK(S)

Lee.J.D. , **A new concise Inorganic Chemistry**, 5th Edition John Wiley & Sons, 2008. (UNIT II & III)

Puri.B.R, Sharma.L.R and Pathania.S., **Principles of Physical Chemistry** , 50th edition , Shoban Lal Nagin Chand & Co., New Delhi, 2011. (UNITS I & IV)

R.D.Madan, **Modern Inorganic Chemistry**, 3rd edition, S. Chand & Company Ltd., 2011. (UNITS II & III)

http://humantouchofchemistry.com/everyday.php?start=30 -21.12.12 (UNIT V)

CHE2101FS DATA HANDLING AND PRESENTATION

(Theory)

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

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

- differentiate the various types of data.
- represent the data using computers.
- write a simple scientific report.

COURSE OUTLINE :

UNIT-I : DATA ANALYSIS **10 Hrs.**

Data- Definition and classification of data- Problem identification – variable - dependent and independent - collection of primary data and secondary data. accuracy, precision, significant figures – measure of central tendency and dispersion Tabulation of data

UNIT-II : DATA REPRESENTATION **10 Hrs.**

conversion of table to graph - Curve sketching - linear (identification of slope and intercept values) and non-linear plots – Using Ms-excel in tabulating data, graphing data – bar charts, pie charts, histograms - errors in presenting graphical data.

UNIT-III : REPORT PREPARATION **10 Hrs.**

Data interpretation - preparation of report – presentation of report (written & oral) – Use of MS Word and Powerpoint in preparing and presenting the report – use of Chemsketch and Marvinsketch for drawing chemical structures - effective usage of internet – plagiarism.

REFERENCE BOOK(S)

Gary D. Christian, **Analytical Chemistry**, 6th edition, John Wiley & Sons, 2011.
Puri.B.R, Sharma.L.R., and Pathania.S, **Principles of Physical Chemistry**, 50th edition, New Delhi, Shoban Lal Nagin Chand & Co, 2011. (Unit I).

WEBSITE(S) :

http://www.microsoft.com/en-us/download/details.aspx?id=30388
http://resources.woodlands-junior.kent.sch.uk/maths/data.htm(UNITII)
http://www.ncl.ac.uk/undergraduate/modules/module/CHY1401/(UNITII)
www.au.af.mil/au/awc/awcgate/army.../graphical-excellence.ppt (UNIT III)

CHE2501CM CHEMISTRY OF ALIPHATIC HYDROCARBONS

(Theory)

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

- acquire the knowledge on the basic concepts of reaction mechanisms
- illustrate the mechanisms involved in alkanes, alkenes, alkynes and alkadienes
- formulate a suitable mechanism for reactions of aliphatic hydrocarbons

COURSE OUTLINE :

UNIT-I : FUNDAMENTALS OF ORGANIC REACTIONS MECHANISMS **15 Hrs.**

Electronic displacements, 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-II : ALKANES AND CYCLOALKANES **15 Hrs.**

Alkanes: Introduction - physical properties- preparation - chemical properties-free radical substitution reactions-halogenation (reactivity and selectivity) nitration-sulphonation-chlorosulfonation-oxidation reactions. **Cycloalkanes:**Introduction- Strain in ring compounds-Baeyer's strain theory- preparation-chemical properties, confirmations of cyclohexane

UNIT-III : ALKENES **15 Hrs.**

Introduction-physical properties- preparation- reduction of alkynes- elimination reactions (Saytzeff's and Hofmann's rule), 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 $KMnO_4$, OsO_4, $K_2Cr_2O_7$, Pb $(OAc)_4$, ozonolysis-allylic substitution reactions -polymerization of alkenes.

IT-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)

Bhupinder Mehta, Manju Mehta,, **Organic Chemistry**, 6th Edition, , PHI Learning Private Limited, New Delhi,, 2011

REFERENCE BOOK(S)

Morrison R. T, Boyd R.N, **Organic Chemistry**, 7th edition, New Delhi, Prentice Hall, 2008.

Raj.K.Bansal, **Organic Reaction Mechanisms**, 3rd edition, New Delhi, Tata MCGraw-Hill Publishing Company Limited, 1998.

Sachin Kumar Ghosh, **Advanced General Organic Chemistry**, 2nd, Calcutta, Books and Allied (P) Ltd, 1998.

Soni. P.L, Chawala H.M, **Text book of Organic Chemistry**, 26, Delhi, Sultan Chand, 1994.

CHE2201CP VOLUMETRIC ANALYSIS

(Lab)

LEARNING OUTCOME : **3 Hrs./Wk.**

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

- know the green principles in volumetric analysis
- apply the knowledge to analyze real time samples

COURSE OUTLINE :

EXPERIMENTS/LAB : 45 Hrs.

INTRODUCTION ON GREEN PRINCIPLES IN CHEMICAL LABORATORY WORK.

ACID - BASE TITRATION

Classifying various chemicals as acids/ bases – test using pH paper, pH meter

Preparation of natural indicators

Titration between

- strong acid vs. strong base
- strong acid vs. weak base
- weak acid vs. strong base
- mixture of acids vs. strong base

Determination of

- acidity in various soft drinks
- strength of antacids
- acid value in oils

REDOX TITRATION

- Iodometric titration – Determination of copper sulphate
- Iodimetric titration – Determination of ascorbic acid in citrus fruits
- Permanganimetry - Determination of iron in iron tablets
- Dichrometry - Determination of ferrous ion

COMPLEXOMETRIC TITRATION

- Determination of hardness of water

REFERENCE BOOK(S)

G.H. Jeffery, J. Basset and others, **Vogel's Textbook of Quantitative Chemical Analysis**, 6th, London, ELBS, 2009..

CHE3401CM - INTRODUCTION TO ORGANIC REACTION MECHANISM

(Theory)

LEARNING OUTCOME : 4 Hrs./Wk.

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

- infer the rates of the reactions of alkyl halides using mechanistic details
- identify the aromatic compounds and predict its reactivity
- analyze the mechanistic details of electrophilic and nucleophilic substitution in aromatic compounds

COURSE OUTLINE :

UNIT-I : ALKYL HALIDES **12 Hrs.**

Nomenclature and classification of organic halogen compounds - 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

Concepts for virtual lab:

- Nucleophilic aliphatic substitution
- Elimination - Mechanisms

UNIT-II : CHEMISTRY OF BENZENE AND ITS DERIVATIVES **12 Hrs.**

Concept of 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, nonbenzenoid aromatic compounds.

Benzene and its derivatives: Nomenclature, Structure of benzene - Kekule structure - stability of benzene - reactions of benzene, Alkenyl benzene, allylic and benzylic halides, Arenes - industrial source of alkyl benzenes, reactions of alkyl benzenes - reduction, oxidation, substitution in ring and side chain. Reactions of alkenyl benzenes - substitution, addition, polymerization.

Concept for virtual lab: HOMO, LUMO visualization - Argus Lab

UNIT-III : ARYL HALIDES **12 Hrs.**

Nucleophilic aromatic substitution, unimolecular ,bimolecular displacement , SNAr mechanism, elimination - addition(benzyne) mechanism. Alkyl halides Vs aryl halides.

Concepts for virtual lab: Nucleophilic aromatic substitution mechanisms.

UNIT-IV : AROMATIC ELECTROPHILIC SUBSTITUTION I **12 Hrs.**

General mechanism for electrophilic substitution , arenium ions, Mechanism - halogenations, nitration, Friedal Crafts alkylation - limitation, Friedel crafts acylation -

Friedel Crafts alkylation vs Friedal Crafts acylation - sulphonation.

Concept for virtual lab: Friedel Crafts alkylation/acylation

UNIT-V : AROMATIC ELECTROPHILIC SUBSTITUTION II **12 Hrs.**

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.

Website(s)

www.chemtube3d.com

TEXT BOOK(S)

Jain. M. K., Sharma, S. C, **Modern Organic Chemistry**, Edition: 4th, New Delhi, Vishal Publishing, 2013, Chapters: UNITS I, IV & V.

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

REFERENCE BOOK(S)

Bhupinder Mehta , Manju Mehta, **Organic Chemistry**, First, Newdelhi, PHI Learning Pvt. Ltd, 2005.

Paula Yurkanis Bruice, **Organic Chemistry**, 3rd, Delhi, Pearson education,Inc, 2002.

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

CHE3402 CM BEHAVIOUR OF GASES AND LIQUIDS

THEORY

LEARNING OUTCOME: **4 Hrs / Wk**

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

- recognize and relate the properties of ideal and real gases
- describe the properties of liquids.
- identify and distinguish the types of solutions
- discuss the fundamental aspects of chemical and ionic equilibrium.

COURSE OUTLINE:

UNIT I IDEAL GASES **12 hrs**

General characteristics of gases- parameters of a gas- gas laws- Boyle's law, Charle'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.

Concepts for Virtual Lab

- All laws
- Collision parameters
- Molecular velocities

UNIT II REAL GASES **12 hrs**

Deviation from ideal behavior – Explanation for deviations of van der Waals' equation –limitations – Liquefaction of gases -Critical phenomena- van der Waals equation and critical constants – experimental determination of critical constants - law of corresponding states –methods of liquefaction of gases.

Concepts for Virtual Lab

- Liquefaction of gases

UNIT III LIQUIDS **12 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.

Concepts for Virtual Lab

- Effect of vapour pressure on boiling point
- Surface tension

UNIT IV SOLUTIONS **12 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 and 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.

Concepts for Virtual Lab

- Distillation techniques
- Solvent extraction

UNIT V CHEMICAL EQUILIBRIA **12 hrs**

Reversible reactions- Nature and characteristics of chemical equilibrium -law of mass action-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 - Thermodynamic derivation of law of chemical equilibrium - temperature dependence of equilibrium constant - homogeneous and heterogeneous equilibria -Le Chatelier's principle

IONIC EQUILIBRIA – Recall on acids and bases-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-their 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.

Concepts for Virtual Lab

- Chemical Equilibrium and Le Chatelier's principle

TEXT BOOK(S)

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

Puri B.R, Sharma L.R and Pathania S., **Principles of Physical Chemistry** , 46th edition , Vishal Publishing Co., New Delhi, 2012. Unit IV, Unit V

REFERENCE BOOK:

Atkins.P.W., **Physical Chemistry** , 8th edition , Oxford University Press, New York, 2006.

WEBSITE(S):

http://www.harpercollege.edu/tm-ps/chm/100/dgodambe/thedisk/equil/8perform.htm Unit V
http://amrita.vlab.co.in/?sub=2&brch=193&sim=1255&cnt=1

CHE3501 CM CHEMISTRY of s- AND p- BLOCK ELEMENTS

THEORY 5 Hrs /Wk

LEARNING OUTCOME:

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

- review the properties of hydrogen and hydrides
- compare the various concepts of acids and bases
- recognize the various metallurgical processes
- summarize the characteristics of s- and p- block elements

COURSE OUTLINE:

UNIT I A: HYDROGEN AND HYDRIDES **15 hrs**

Position of hydrogen in the periodic table - resemblance 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.

I B: NON-AQUEOUS SOLVENTS

Classification of solvents – characteristic properties of solvents – liquid ammonia, liquid N_2O_4, liquid sulphur dioxide, liquid hydrogen sulphide, liquid HF.

UNIT II A: METALLURGICAL PROCESSES **15hrs**

Occurrence of metals- steps involved in metallurgical processes – concentration of ore- calcination – roasting – smelting – electrometallurgy – refining - thermodynamics of oxidation of metals to metal oxides – Ellingham diagram.

Concepts for virtual lab

- Elements in periodic table
- Metal extraction- Alloy analysis: (Sn, Pb, Fe, Cu and Zn)

II B: s- BLOCK ELEMENTS

General characteristics and periodicity in the properties of groupI 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

Concepts for virtual lab

- Flame test- s block elements
- Reaction of Na with water

UNIT III A .BORON GROUP **15 hrs**

Comparison of Boron and Aluminium- compounds- Boron trioxide- Boric acid and their salts, boron nitride- borazine – Boranes- structure and bonding in B_2H_6 and B_4H_{10}- alumina, aluminium chloride

Concept for virtual lab

- Bonding in boranes

III B. CARBON GROUP

Anomalous behaviour of carbon- comparison of carbon and silicon-allotropy of carbon- diamond, graphite, fullerene and graphene - intercalation compounds of graphite- structure of oxides, oxyacids and their salts- percarbonates, perhydrates of carbonates- carbides classification- silica, classification, structure – silicates.

Preparation, properties- Stannous chloride - white and red lead.

Concepts for virtual lab:

- Allotropes of carbon
- Intercalation of graphite
- Silicates

UNIT IV A. NITROGEN GROUP **15 hrs**

Difference between Nitrogen and other elements- active nitrogen – structure and properties of hydrides-classification of nitrides - structure and properties of oxides, oxoacids of nitrogen–(N_2O, NO, N_2O_4, N_2O_5, HNO_2, HNO_3) and phosphorus - (H_3PO_4, H_3PO_3)- halides of phosphorus- PCl_3, PCl_5- polysulphides of phosphorus- phosphazines- classification- Distinction between sulphides of As, Sb, Bi.

IV B. OXYGEN GROUP

Anomalous behaviour of oxygen- oxides and their classification- ozone- preparation, properties, formula- hydrogen peroxide – polysulphide ions-comparitive study of hydrides- structure and properties of oxides (SO_2 and SO_3) and oxoacids of sulphur- (H_2SO_4, peroxosulphuric acid, thionic acids) - structure of halides of sulphur.

UNIT V A. HALOGEN FAMILY **15 hrs**

Anomalous behaviour of fluorine- comparative study of halogen acids and halides- structure of halogen oxides, oxoacids- interhalogen compounds- ICl, BrF_3, IF_5, IF_7-polyhalides- pseudohalogens – cyanogen- pseudohalides – comparison of halogens and pseudo halogens.

V B. NOBLE GASES

Discovery- position in the periodic table- periodicity - separation and isolation of noble gases- general properties and uses- compounds of noble gases- xenon fluorides – structure & properties- clathrates.

TEXT BOOK(S)

Puri B.R., Sharma L.R., Kalia K.C, **Principles of Inorganic Chemistry**, 31st edition, Milestone Publishers and distributors, Delhi, 2010.

REFERENCE BOOK(S)

Atkins P., Overton T., Rourke J.,Weller M., Armstrong. F., **Shriver & Atkins' Inorganic Chemistry,** 4th edition, Oxford University Press, New Delhi, 2006.

Lee.J.D., **A New Concise Inorganic Chemistry** , 5th edition, ELBS, London, 2002.

Madan.R.D., **Modern Inorganic Chemistry**, 3rd revised edition, S.Chand and company, New Delhi, 2011.

WEBSITE(S) :

http://www.theodoregray.com/periodictable/AlkaliBangs/index.html

http://amrita.vlab.co.in/?sub=2&brch=193&sim=1255&cnt=1

http://www.800mainstreet.com/spect/emission-flame-exp.html#Anchor-ca

http://dqino.ua.es/en/virtual-lab/virtual-lab.html

http://www.chemeddl.org/resources/top10.php

http://ocw.mit.edu/courses/chemistry/

CHE3201 CP EXPERIMENTAL PHYSICAL CHEMISTRY

(LAB COURSE)

LEARNING OUTCOME: **3 Hrs/Wk**

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

analyze and interpret the experimental data.
validate the theoretical concepts through experiments.
design an indigenous experiment based on the concepts.

CORUSE OUTLINE:

Concept & Experiment	Hours
Viscosity of liquids	3
1. Determination of viscosity of oils/ milk / solvents using Ostwald's Viscometer.	
Refractive index of liquids	3
2. Specific and Molar Refraction of a Liquid by Abbe's Refractometer.	
Optical activity	3
3. Determination of specific rotation of sucrose solution by Polarimeter.	
Miscibility of liquids	3
4. Critical solution temperature of partially miscible liquid system.	
5. Effect of electrolytes on CST	
Partition coefficient	6
6. Partition coefficient for the distribution of Iodine between water and CCl_4	
Buffers	6
7. Preparation of buffer mixtures	
8. Determination of pH of various Buffer mixtures	
Acid-base indicators, pH-Acidity vs. alkalinity	3
9. Determination of working range of indicators	3
10. pH titration of a mixture of acids (strong and weak) with a strong base.	
Dissociation constant	3
11. Determination of dissociation constant of organic acids.	
Solubility, solubility product and Common ion effect	6
12. Determination of solubility , solubility product of sparingly soluble salts	
13. Study on the effect of common ion on the solubility of sparingly soluble salts.	
Degree of hydrolysis	3
14. Determination of hydrolysis constant of salts of acids and bases (any one of the four types)	
One self design experiment by the student based on any one of the above concepts	3

REFERENCE BOOK(S):

Ahluwalia V.K., Sumitha Dingra and Adarsh Gulati, **College Practical Chemistry**, University Press Pvt Ltd.,Hyderabed, India, 2005

Gary D. Christian, **Analytical Chemistry,** Sixth edition, John Wiley & Sons, Kundli, 2011

Peter Mathews G., **Experimental Physical Chemistry**, Clarendon Press Oxford, 1985.

Viswanathan B., Raghavan, P. S. **Practical Physical Chemistry,** Viva books Private limited, Newdelhi 2012.

CHE 0301 CP EXPERIMENTAL ORGANIC CHEMISTRY LAB COURSE

III SEM : 3 Hrs / Wk
IV SEM : 3 Hrs / Wk

LEARNING OUTCOME:

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

- analyse the functional groups present in the given organic compound.
- synthesize industrially important compounds.
- apply the green principles in the preparation of organic compounds.

COURSE OUTLINE:

I. REACTIONS

Study of the effects on the rates of S_N2 reactions **5 hrs**

a. Structure of the Alkyl Halide

b. Steric Effects

c. Leaving Group

II. ORGANIC SYNTHESIS **8 hrs**

a. Synthesis of Phenacetin; The Williamson Ether Synthesis

b. Synthesis of Diazonium Dyes

III. GREEN SYNTHESIS **8hrs**

a. Aldol condensation/Benzoin Condensation

b. Benzilic acid rearrangement

IV. QUALITATIVE ANALYSIS OF THE FOLLOWING ORGANIC COMPOUNDS **70hrs**

Identification of nature and elements present

Preparation of derivatives

- Phenol
- Aldehydes
- Ketones
- Carboxylic acids
- Esters
- Nitro compounds

- Amine
- Amide
- Diamide
- Carbohydrates (mono- and di-saccharides)

REFERENCE BOOK (S):

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

Furniss B.S.et al, **Vogel's Textbook of Organic Chemistry**, ELBS, 5th edition, London, 1989.

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

WEBSITE(S) :

http://www.umsl.edu/~orglab/

CHE 4401CM CHEMISTRY OF ORGANIC COMPOUNDS WITH OXYGEN FUNCTIONALITY (THEORY)

LEARNING OUTCOME: **4 Hrs / Wk**

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

summarize the reactivity of alcohols , phenols, ethers and epoxides.

illustrate the condensation reactions of aldehydes and ketones

asses the chemistry of aliphatic and aromatic carboxylic acids and its derivatives.

compare the acidic properties of carboxylic acids, substituted carboxylic acids and phenols.

COURSE OUTLINE:

UNIT- I: ALCOHOLS, PHENOLS, ETHERS AND EPOXIDES:

12 hrs

Alcohols: Physical properties – alcohols as an acid and as a base – reactions involving the acidic and basic characteristics of alcohols - relative reactivity of 1^0, 2^0, 3^0 alcohols and distinction- ascent and descent in alcohol series, comparison of alcohols with thiols

Phenols: Preparation and properties; Acidity and factors affecting it, Ring substitution reactions, Reimer – Tiemann and kolbe–schmitt reaction, Fries and Claisen, Lederer - Manasse reaction, rearrangements with mechanism-reactions of analytical importance.

Ethers: Preparation – Williamson ether synthesis, alkoxy mercuration and demercuration of alkenes – reactions involving etheral oxygen and ether linkage – comparison of ethers with thioethers, crown ethers (introduction only)

Epoxides: Ring opening reactions of epoxides

Concept for virtual lab:

Reactions of alcohols and phenols

UNIT –II: ALIPHATIC AND AROMATIC CARBONYL COMPOUNDS :

12 hrs

Structure and reactivity of carbonyl group – nucleophilic addition reactions – reaction with carbon nucleophiles – oxygen nucleophiles , nitrogen nuclephiles, 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

Concept for virtual lab:

Analytically important reactions of carbonyl compounds

UNIT- III : REACTIONS OF ALDEHYDES AND KETONES:

12 hrs

Acidity of α 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, Cannizaro's reaction- Crossed Cannizzaro reaction, Mannich reaction, Wittig reaction - Reactions of α, β – unsaturated compounds- Michael addition, Perkin, Knoevenagel, Stobbe condensations – Benzilic acid rearrangement.

UNIT -IV: ALIPHATIC AND AROMATIC CARBOXYLIC ACIDS AND THEIR DERIVATIVES:

12 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 sustitution at acyl group - Mechanism of acidic and alkaline hydrolysis of esters, Dieckmann and Reformatsky reactions, Hofmann-bromamide degradation and Curtius rearrangement, Sulphonic acid

Concept for virtual lab:

Reactions of carboxylic acids and its derivatives.

UNIT -V UNSATURATED AND SUBSTITUTED CARBOXYLIC ACIDS:

12 hrs

Acidity of substituted acids, Typical reactions of dicarboxylic acids, keto acids , hydroxy acids and unsaturated acids: succinic/,lactic, malic, tartaric, citric, maleic, fumaric and cinnamic acid , salicylic acid, phthalic acid.

TEXT BOOK (S):

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

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

REFERENCE BOOK(S):

Bhupinder Mehta , Manju Mehta, **Organic Chemistry,** First edition**,** PHI Learning Pvt. Ltd., Delhi ,2005.

Morrison R. T, Boyd R.N., **Organic Chemistry** , 7th edition , Prentice Hall, New Delhi, 2008.

Solomons T.W.G., **Organic Chemistry**, 8th edition, John Willey & Sons Inc., Singapore, 2004

WEBSITE(S):

www.**chemtube3d**.com

CHE4402CM CHEMISTRY OF TRANSITION ELEMENTS

THEORY

4Hrs/Wk

LEARNING OUTCOME:

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

- recognize 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 OUTLINE:

UNIT I: INORGANIC POLYMERS & NANO MATERIALS 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- organosilicones- preparation- structures- applications.

Introduction - definition for nanodimensional material (particles, rods, wires, tubes with examples) – metallic nanoparticles- gold and silver –method of preparation (Chemical reduction method)and applications. Carbon Nanotubes - types, SWCNT, MWCNT – method of preparation –applications.

Concepts for virtual lab:

- Preparation of CNT
- Synthesis of silver and gold nano particles

UNIT II: GENERAL CHARACTEREISTICS OF d-BLOCK ELEMENTS 12 hrs

General properties- size- density- melting point- boiling point- reactivity of metals- ionisation potentials- colour- magnetic properties- paramagenetism, diamagenetism, ferromagenetism, antiferromagenetism – 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.

Concept for virtual lab

Magnetic properties

UNIT III: FIRST TRANSITION SERIES 12 hrs

Preparation, properties and uses - **Titanium compounds** - titanium dioxide, titanium tetrachloride – **Chromium compounds**- chromous acetate, 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.

Concept for virtual lab

Colour reactions of Cr, Fe, Ni and Cu

UNIT IV: SECOND AND THIRD TRANSITION SERIES 12 hrs

Preparation, properties and uses **- Molybdenum compounds**- molybdenum blue, Ammonium molybdate— 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.

Concept for virtual lab

- Colour reactions of Mo and Hg

UNIT V: 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.

Concept for virtual lab

Lanthanide contraction

TEXT BOOK:

Puri B.R., Sharma L.R., Kalia K.C, **Principles of Inorganic Chemistry**, 31st edition, Milestone Publishers and distributors, Delhi, 2010.

REFERENCE BOOK(S):

Atkins P., Overton T., Rourke J.,Weller M., Armstrong. F. Shriver & Atkins' **Inorganic Chemistry,** 4th edition, Oxford University Press, New Delhi, 2006.

Lee.J.D., **A New Concise Inorganic Chemistry** , 5th edition, ELBS, London, 2002. (UNIT II, III, IV &V)

Pradeep T., **Nano: The Essentials**, McGraw Hill Education, New Delhi, 2009. (UNIT I)

CHE4403 CM INTRODUCTION TO CHEMINFORMATICS (THEORY)

4 Hrs/Wk

LEARNING OUTCOME:

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

- recognize the different types of 2D and 3D molecular representations
- identify the database models
- describe the applications of various databases
- classify the various datamining techniques

COURSE OUTLINE:

UNIT I: CHEMICAL REPRESENTATION OF MOLECULES 12hrs

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, Sdfiles 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: DATABASE DESIGN & THEIR MANAGEMENT 12hrs

Database Concepts- Structure Query Language, Design of Chemical Databases, Data Abstraction; Data Models; Instances & Schemes; E-R Model - Entity and entity sets; Relations and relationship sets; E-R diagrams; Reducing E-R Diagrams to tables; Network Data Model: Basic concepts; Hierarchical Data Model: Basic Concepts; Metadatabases; Indexing and Hashing; Basic concepts; Text Databases; Introduction to Distributed Database Processing, Data Security. Interfacing programs with databases

UNIT III: DATABASES 12 hrs

Sources, contents, design, Accessibility and use-**Chemical database**-PUBCHEM, CHEMBANK, DRUGBANK, JCHEM, IUPAC, CAS Registry, ZINC, MOLTABLE, ChemExper, ChemSpider-**Literature database**-PUBMED-**Biological database-**PRIDE**,** chemPDB, KEGG, Ligand Info, GenBank, NCI

UNIT IV: DATAMINING AND CHEMICAL STRUCTURE SEARCHING 12hrs

Datamining: **Introduction** – Aspects of data mining-Techniques of Data mining – Multi dimensional models – cube – star – snowflakes – classification techniques – K-nearest neighbour – Decision tree — Bayesian classifier – Introduction to neural network.

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.

UNIT V: COMBINATORIAL CHEMISTRY: 12 hrs

Principle of combinatorial chemistry – synthesis methods- Split-mix, parallel- diversed and focused libraries- library enumeration- combinatorial library design stratergies- approaches to product based library design-Molecular Scaffolds- Rule of five, Druglikeliness, Leadlikeliness, Drug design and combinatorial libraries– case studies.

TEXTBOOK(S):

Johann Gasteiger **(ed.),** Thomas Engel **(ed.), Chemoinformatics: A Textbook, Wiley VCH,** Weinheim **2003. (Unit I,IV)**

Jiawen Han and Micheline Kamber, **Data Mining-Concepts and Techniques**, Second Edition, Elsevier publication, 2006. (Unit IV)

Leon A. & Leon M., **Database Management System**, Vikas Publishing House, Chennai, 2002.(Unit II)

REFERENCE BOOK(S):

Andrew R. Leach, Valerie J. Gillet. **An Introduction to Chemoinformatics, revised edition, Springer, Netherland, 2007.**

Larsen **Textbook of Drug Design and Discovery**, 3rd edition, Taylor and Francis, London and New York, 2004.

CHE4501CM CHEMICAL THERMODYNAMICS

THEORY

LEARNING OUTCOME: 5 Hrs / Wk

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

- classify the various types of solids based on symmetry elements.
- correlate the type of colloids with its properties.

- identify the fundamental concepts of thermodynamics
- relate and interpret the various laws of thermodynamics
- recognize the terms involved in statistical thermodynamics

COURSE OUTLINE:

UNIT I: FIRST LAW OF THERMODYNAMICS **15 hrs**

Terms and concepts-systems, boundary, surroundings-macroscopic properties-intensive and extensive-state variables-thermodynamic processes-reversible and irreversible processes-nature of work and heat-pressure-volume work, isothermal, reversible and irreversible expansion, work done in reversible expansion, internal energy- first law of thermodynamics-enthalpy of a system-molar heat capacity-Joule Thomson effect-adiabatic expansion and work done.

UNIT II: THERMOCHEMISTRY **15 hrs**

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.

Concepts for Virtual Lab

- Fundamentals of thermodynamics(different processes)
- Joule Thomson experiment
- Phase transition and energy change
- Bomb calorimeter

UNIT III: SECOND LAW OF THERMODYNAMICS I **15hrs**

Limitations of the first law-Spontaneous processes and criteria of spontaneity-entropy-second Law – Standard Entropy, entropy of formation, cyclic processes, heat engine , efficiency-Carnot cycle-carnot theorem, other forms of second law- entropy from Carnot cycle- entropy change - irreversible process, for an ideal gas, during change of phase, free energy-free energy and work function, variation of free energy with temperature and pressure, isothermal change in free energy, Gibbs- Helmholtz equation and its importance-Criterion for a spontaneous process

Concepts for Virtual Lab

- Spontaneous/ non spontaneous processes
- Entropy change
- Carnot cycle

UNIT I V SECOND LAW OF THERMODYNAMICS II **15 hrs**

Clausius Clapeyron equation and its application- van't Hoff isotherm and isochore, derivations of expressions for lowering of vapour pressure, osmotic pressure, elevation in boiling point and depression in freezing point- fugacity and activity, chemical potential and its physical significance- Gibbs-Duhem equation-Third Law of thermodynamics-Nernst heat theorem-third law of thermodynamics-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.

Concepts for Virtual Lab

- Colligative properties
- Probability and statistics
- Micro and macro states
- Ensembles

UNIT V: STATISTICAL THERMDYNAMICS **15 hrs**

Introduction to Statistical Thermodynamics- macro and micro states- ensembles- thermodynamical probability according to Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics-most probable distributions.

COLLOIDAL STATE

Colloids – types of colloids – lyophillic 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.

Concepts for Virtual Lab

Peptization, Electrodialysis, electro osmosis, coagulation, surfactants, cleaning action of soaps and detergents, emulsion, gels, ultramicroscope, Tyndall effect, Brownian movement .

TEXT BOOK(S):

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

REFERENCE BOOK(S):

Atkins.P.W, **Physical Chemistry**, 8h edition, Oxford University Press, New York, 2006.

Puri.B.R, Sharma.L.R and Pathania.S., **Principles of Physical Chemistry** , 46th edition , Vishal Publishing

Co., New Delhi, 2012.

WEBSITE(S) :

http://amrita.vlab.co.in/?sub=2&brch=193&sim=1255&cnt=1

CHE4201CP EXPERIMENTAL INORGANIC CHEMISTRY

LAB COURSE

3Hrs/Wk

LEARNING OUTCOME:

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

- identify the acid and basic radicals
- analyse the salt mixture qualitatively
- discuss the physico-chemical principles involved in the analysis

COURSE OUTLINE:

SEMI MICRO ANALYSIS INVOLVING GREEN PRINCIPLES

Qualitative analysis of Acid radicals

- CO_3^{2-}, NO_3^-, CH_3COO^-, Cl^-, Br^-, I^-, SO_4^{2-}, PO_4^{3-}, BO_3^{3-},F^-, $C_2O_4^{-2}$, CrO_4^{2-}, $S_2O_3^{2-}$,
- $C_4H_4O_6^{2-}$

- Qualitative analysis of 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^+
- Qualitative analysis of salt mixture – Analysis of a salt mixture containing three anions and three cations, inclusive of rare earths with atleast one interfering anion.

REFERENCE BOOK(S):

Jeffery, G.H.. Basset J and others, **Vogel's Textbook of Quantitative Chemical Analysis**, ELBS, 5th edition, London, 1989.

Pass G. & Sutcliffe H., **Practical Inorganic Chemistry**, 2nd edition, Chapman & Hall Ltd, London, 1979.

Ramanujam V.V., **Inorganic Semi Micro Qualitative Analysis**, The National Publishing Company, Chennai, 1990.

WEBSITE(S) :

http://web.mst.edu/~gbert/qual/qual.html

http://www.dartmouth.edu/~chemlab/chem3-5/qual_cat/full_text/procedure.html

http://www.dartmouth.edu/~chemlab/chem3-5/qual_an/overview/procedure.html

CHE4201SP CHEMINFORMATICS LAB

2

Hrs/Wk

LEARNING OUTCOME:

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

apply the datamining tools

COURSE OUTLINE:

	Experiments	**Hrs**
1.	Construction of molecules in Argus Lab, BKTool, ChemSketch and MarvinSketch	6
2.	Energy Optimization of the Built molecule	2
3.	Retrieving the SMILES notation of the molecules	2
4.	Converting the molecules into different file formats	2
5.	Analysis of the molecular surfaces and molecular orbital of small molecules, proteins and nucleic acids using MarvinSpace	4
6.	Representation of reactions in MarvinView	4
7.	Creation of a database table using SQL commands	2
8.	Determination of HOMO/LUMO band gap energy in benzene	2
9.	Application of datamining- WEKA	4
10.	Demonstration of CombiChem lab	2

TEXT BOOK:

Donald L. Pavia, Gary M. Lampman, George S. Kriz & Randall G. Engel, **Organic Chemistry A Lab Manual**, Cengage Learning, 2009

CHE 5201 CP ADVANCED EXPERIMENTAL CHEMISTRY

LAB COURSE

3hrs/W

k

LEARNING OUTCOME:

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

- analyze and interpret the experimental data.
- validate the theoretical concepts through experiments.

1. **Chemical kinetics** – Determination of order of a reaction – Hydrolysis of ester, Inversion of sucrose.
2. **Adsorption** – Adsorption of dye onto adsorbents.
3. **Photochemistry** – Verification of Beer-Lambert's law
4. **Electrochemistry** – Determination of standard reduction potential.
   - Potentiometric redox titrations.
   - Conductometric titration of an acid and a base.
5. **UV Visible Spectrophotometry-** Spectrophotometric determination of
   Ferrous ions by using 1,10 phenanthroline
   Ni^{2+} by complexing with DMG
6. **Flame photometry-** Determination of Na, Ca, Li in cola drinks and fruit juices
7. **Atomic absorption Spectrophotometry-**Determination of Ca/Mg in drugs
8. **Synthesis and characterization of**
   tetraammine copper (II) sulphate, $[Cu(NH_3)_4]SO_4\ H_2O$
   pentaammine carbonato Cobalt (III) ion

REFERENCE BOOK(S):

Ahluwalia V.K., Sumitha Dingra and Adarsh Gulati, **College Practical Chemistry**, University Press Pvt Ltd.,

India, 2005

Day R. A., Underwood A. L., **Quantitative analysis**, Prentice Hall of India Pvt., Ltd., 2003, sixth edition.

Gary D. Christian, **Analytical Chemistry,** John Wiley & Sons, 2011 , Sixth edition.

Gurtu J.N and Kapoor. R., **Advanced Experimental Chemistry,** S. Chand & Co., New Delhi, 1989.

Pass G. & Sutcliffe H., **Practical Inorganic Chemistry, preparations, reactions and instrumental methods**, Chapman and Hall ltd, 1979, second edition.

Viswanathan B.,. Raghavan P. S., **Practical Physical Chemistry,** Viva books Private limited, 2012.

WEBSITE(S):

http://www.dartmouth.edu/~

http://amrita.vlab.co.in/

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.

CHE5401CM COORDINATION AND BIOINORGANIC CHEMISTRY

(THEORY)

LEARNING OUTCOME: **5 HRS./WK.**

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

- Recognize the basic concepts of co-ordination chemistry
- Review the importance of metallobiochemistry and identify the role of metals in medicine
- Describe the chemistry of carbonyls and nitrosyls
- Relate the structure, electrical and mechanical properties of solids

COURSE OUTLINE :

UNIT-I : CO-ORDINATION CHEMISTRY I **15 HRS.**

Introduction- werner's theory- types of ligands- nomenclature- isomerism-stability of complexesbonding in complexes- vbt- cft- strong and weak ligands-nephelauxetic effect - mot as

applied to octahedral complexes- spectrochemical series- comparison of vbt, cft & mot - jahn-teller effect.

CONCEPTS FOR VIRTUAL LAB:

Crystal field theory

UNIT-II : CO-ORDINATION CHEMISTRY II **15HRS.**

Spectral and magnetic properties of metal complexes- term symbols- electronic spectra of Complexes (d^1 and d^9)- electronic absorption spectrum of [ti $(h_2o)_6]^{3+}$ 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.

Concepts for virtual lab:

Magnetic behaviour

UNIT-III : BIO- INORGANIC CHEMISTRY **15 HRS.**

Role of alkali and alkaline earth metals in biological systems-na+/k+ pump - role of hemoglobin and myoglobin in biological systems - biological functions and toxicity of cr, mn, fe, co, cu, mo, zn - nitrogen fixation.

CONCEPTS FOR VIRTUAL LAB:

Role of hemoglobin

Nitrogen fixation

UNIT-IV : CARBONYLS AND NITROSYLS **15 HRS.**

Carbonyls- classification – general methods of preparation – properties- structure and bonding – mononuclear carbonyls, binuclear carbonyls- cr $(co)_6$, fe $(co)_5$, ni $(co)_4$, mn_2 $(co)_{10}$, co_2 $(co)_8$, $fe_2(co)_9$- 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.

CONCEPTS FOR VIRTUAL LAB

Structure and bonding in carbonyls

UNIT-V : SOLID STATE **15 HRS.**

Types of solids – isotropy and anisotropy – symmetry of crystals – miller indices – crystal structure – cubic unit cells – x-ray crystallography – bragg's equation – measurement of diffraction angle – 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.

CONCEPTS FOR VIRTUAL LAB

Crystal structures

TEXT BOOK(S)

Lee.j.d .,, *a new concise inorganic chemistry*, 5th edition, london,: elbs, 2002. Print.

Puri.b.r, sharma.l.r & kalia.k.c,*principles of inorganic chemistry*, 31st edition, new delhi: Vallabh publications, 2013. Print.

REFERENCE BOOK(S)

Atkins p., overton t., rourke j.,weller m., armstrong. F., *shriver& atkins'inorganic chemistry*, 4th edition, new delhi: oxford university press, 2006. Print.

Azaroff. L.,*introduction to solids*, new delhi: tata mcgraw hill publishing company, 1995. Print.

Madan.r.d.,*modern inorganic chemistry*, new delhi: s.chand & sons, 1987. Print.

Malik. U, madan.r.d and tuli.g.d.,*selected topics in inorganic chemistry*, new delhi: s.chand & company, 2007. Print.

WEBSITE(S) :

Http://amrita.vlab.co.in/index.php?sub=2&brch=193&sim=610&cnt=1

CHE5502CM CHEMICAL KINETICS, CATALYSIS AND ELECTRO CHEMISTRY (THEORY)

LEARNING OUTCOME : **5 HRS./WK.**

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

- Describe the kinetics of chemical reactions.
- Identify the different types of adsorption.
- Explain the characteristics of catalysis.
- Predict the electrochemical properties of a cell reaction.

COURSE OUTLINE :

UNIT-I : CHEMICAL KINETICS I **15 HRS.**

Rate law- rate measurements-factors affecting rates of reactions-order and molecularity of a reaction-zero, first, second, third and fractional order reactions-methods of following kinetics and order of reactions-temperature dependence of rate constants-arrhenius equation-determination of activation energy.

CONCEPTS FOR VIRTUAL LAB:

Activation energy

UNIT-II : CHEMICAL KINETICS II AND SURFACE CHEMISTRY **15 HRS.**

Theories of reaction rates-collision theory of gaseous bimolecular reactions-unimolecular reactions-lindemann hypothesis-equilibrium approximation-steady state approximation-limitations of collision theory- arr theory. Adsorption-types of adsorption - physisorption and chemisorptions – adsorption of gases by solids-factors affecting adsorption, adsorption isotherms-different types of adsorption isotherms-freundlich and langmuir isotherms-applications of adsorption.

CONCEPTS FOR VIRTUAL LAB:

Collision theory.

Adsorption isotherm.

UNIT-III : CATALYSIS **15 HRS.**

Catalysis-general characteristics of catalytic reactions, promoters, catalytic poisoning, Autocatalysis, negative catalysis, activation energy and catalysis, types of catalysis -homogenous -acid-base catalysis -and enzyme catalysis- michaelis – menten effect of temperature and ph in Enzyme catalysis-heterogeneous catalysis-surface reactions – langmuir-hinshelwood mechanism, unimolecular and bimolecular surface reactions.

CONCEPTS FOR VIRTUAL LAB:

Types of chemical catalysis

Enzyme catalysis

Surface reactions

UNIT-IV : ELECTROCHEMISTRY - I **15 HRS.**

Types of conductance-electrolytic, specific, molar, equivalent - cell constant- variation of molar Conductance with concentration - ionic mobility-transport number- kohlrausch's law and its Applications- diffusion and ionic mobility- applications of conductance measurements-arrhenius Theory-ostwald's dilution law- debye-huckel theory of strong electrolytes-debye-falkenhagen and wien effect.

CONCEPTS FOR VIRTUAL LAB:

Diffusion and ionic mobility

UNIT-V : ELECTROCHEMISTRY II: **15 HRS.**

Half reactions-oxidation and reduction, electrochemical cells-galvanic and electrolytic cellsreversible cells-types of electrodes- ag-agcl, hydrogen, calomel, glass, quinhydrone electrodes- emf-calculation of emf of a cell, cell representation –emf and free energy-standard emfstandard electrode potentials, ELECTROCHEMICAL SERIES, nernst equation, application of emf measurement-potentiometric titrations, solubility of sparingly soluble salt- concentration cells.

CONCEPTS FOR VIRTUAL LAB:

Emf of the cell

Gibbs free energy change

Equilibrium constant

Spontaneity of the cell reaction

TEXT BOOK(S)

Arun bahl, b.s. bahl and g.d.tuli, *essentials of physical chemistry*, new delhi,: s.chand and co. Ltd, 2009. Print.

Puri.b.r, sharma.l.r and pathania.s, *principles of physical chemistry*, 46th edition., jalandhar:

Vishal publishing co., 2012. (units i,iii,iv), print.

WEBSITE(S) :

WWW.EVICAB.EU/BME/06MALMI/VIDEO/FRAME/10.HTM

CHE5501CM NITROGEN COMPOUNDS AND NATURAL PRODUCTS

(Theory)

LEARNING OUTCOME : **5 Hrs./Wk.**

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

- acquire the knowledge on the reactions of amines and nitro compounds
- describe the properties of heterocyclic compounds.
- recognize the structure and properties of biomolecules
- analyse the structure and properties of natural products.
- summarize the characteristics of carbohydrates.

COURSE OUTLINE :

UNIT-I : AMINES AND NITRO COMPOUNDS **15 Hrs.**

Amines: Preparation and properties- Hofmann – Martius rearrangement , Fischer-Hepp rearrangement, Diazoamino-aminoazo rearrangement, Benzidine rearrangement, Lossen rearrangement, Schmidt reaction, Hofmann's exhaustive methylation,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 1º, 2º and 3º 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 : HETEROCYCLIC COMPOUNDS: **15 Hrs.**

Introduction, nomenclature, five membered rings, preparation& structure of furan, pyrrole , electrophilic substitution- reactivity and orientation, derivatives, Knorr-pyrrole synthesis, Paal-Knorr synthesis, Indole – Fischer Indole syntheis, six membered rings- pyridine – synthesis, structure, basicity of pyridine, electrophilic substitution, nucleophilic substitution, Chichibabain reaction, methods of ring fission- piperidine. Self study-Thiophene.

Concept for Virtual Lab:

Structure and reactions of heterocyclic compounds

UNIT-III : POLYNUCLEAR HYDROCARBONS **15 Hrs.**

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

UNIT-IV : ALKALOIDS AND TERPENOIDS **15 Hrs.**

Alkaloids: Definition - extraction - general properties – general methods of determining structure – classification , structural elucidation and synthesis of

pyridine & piperidine group – piperine,

pyridine &pyrrolidine group – Cocaine.

Terpenoids: Introduction - classification - isolation - isoprene rule and special isoprene rule- general methods of determining the structure,structure and synthesis of Acyclic – citral Bicyclic – camphor.

Concept for Virtual Lab:

Extraction of alkaloids

UNIT-V : 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 at anomeric carbon, methylation, determination of ring size. conformations of glucose, disaccharides – general study of cellobiose, sucrose,(structure and specific properties)- Haworth structure.

TEXT BOOK(S)

Jain. M. K., Sharma, S. C,, **Modern Organic Chemistry**, 4, New Delhi: Vishal Publishing, 2013.

Morrison R. T, Boyd R.N, **Organic Chemistry**, 7, New Delhi: Prentice Hall, 2008.

REFERENCE BOOK(S)

Agarwal .O.P., **Chemistry of natural products - Vol. II**, 32nd Edition, Meerut,, Goel Publishing House, 2007.

Chatwal Gurdeep, **Chemistry of natural products - Vol. II**, 5th Edition., Delhi, Himalaya publishing House, 2008.

Finar I.L., **Organic Chemistry – Vol. I & II**, 8th Edition., Pearson Education, 2011,.

Mehta, B. Mehta, M, **Organic Chemistry**, 1st edition, , Delhi, PHI Learning Pvt. Ltd, 2005.

WEBSITE(S) :

http://www.chemtube3d.com/HeterocyclicTitle%20page.html

CHE0601LM WATER QUALITY MANAGEMENT

LEARNING OUTCOME:

on successful completion of the life frontier engagement programme the student will be able to

- Evaluate the level of pollution in a water body
- Assess the quality of water through standard procedures
- Suggest suitable strategies to recycle and recharge water.
- offer suitable solutions for the community with water related issues.

THE COMMUNITY BASED ACADEMIC LEARNING PROCESS WILL BENEFIT THE STUDENTS TO

- Learn the various methods adopted by the community to address the water related issues
- Gain a hands-on practical experience on the theoretical concepts

PROJECTED BENEFITS OF COMMUNITY PARTNERS:

THE COMMUNITY PARTNERS WILL BE ABLE TO

Imbibe and sensitize the importance of water in life

Appreciate and apply the strategies and solutions to solve water related issues

SECTION II –THEMATIC CONCEPTS **15 HRS.**

- **WATER POLLUTION**
- **WATER QUALITY ANALYSIS**
- **WATER CONSERVATION**

1. WATER POLLUTION – DESCRIBED BASED ON THEORETICAL AND CLASSIFICATIONAL CONCEPTS

THEORETICAL CONCEPT

The main causes for water pollution are the following

- Contamination of water bodies due to increase in population, human intervention, industrialization, and oil spillage.
- Shrinkage and depletion of natural water reservoirs.
- excessive construction of concrete buildings.

CLASSIFICATIONAL CONCEPT

The types of water pollution are classified based on the

- Sources of water – surface water, oceanic, and underground water pollution,
- nature of pollutants - natural sources (land destructin, humus, gas), human sources (agriculture, industry, domestic), effluents (thermal, oil, sewage water etc)
- Type of pollution – physical, chemical, organic, physiological pollution

2. WATER QUALITY ANALYSIS –DESCRIBED BASED ON CLASSIFICATIONAL AND CO-RELATIONAL CONCEPTS

CLASSIFICATIONAL CONCEPT

- Water quality analysis is broadly classified as physical and chemical analysis.
- Comparison of the analyzed data with the permissible limits as the required standards.
- Assessment of the water quality based on the result obtained.

CO-RELATIONAL CONCEPT

The quality of the water sample and its suitability can be assessed based on the various physical and chemical parameters in comparison with the water quality standards.

3. WATER CONSERVATION - DESCRIBED BASED ON CO-RELATIONAL CONCEPT

If water is judiciously used, recycled appropriately, harvested effectively during seasonal rainfalls, then it can be conserved for the future generation.

THE FOLLOWING ARE THE ACTIVITIES AND THE METHODOLOGIES FOR THE ABOVE THREE SUBTHEMES IDENTIFIED

1. **SUB THEME**: WATER POLLUTION

EXPECTED OUTCOME: THE ACTIVITIES WILL ENABLE THE STUDENT TO

- Classify the types of pollution in a water body
- Know the different methods of prevention of pollution

ACTIVITY:

(I) case study presentation

METHODOLOGY: the students will collect case studies through different resources (media and internet) and discuss the issues related to water pollution prevailing all over the world.

(ii) group discussion

METHODOLOGY: the students will discuss in groups to reflect upon the prevalent water related problems in the local community

(III) MODEL MAKING / CHART PREPARATION/ SHOT FILM/ VIDEO CLIPPINGS

METHODOLOGY: the students will depict the various sources of water pollution and methods of prevention through

Appropriate method.

(iv) article preparation

METHODOLOGY: the students will prepare and present an article on water pollution

2. **SUB THEME**: WATER QUALITY ANALYSIS

EXPECTED OUTCOME

THE ACTIVITIES WILL ENABLE THE STUDENT TO

- Learn the standard procedures for water quality analysis
- Assess the water quality based on a given data

ACTIVITY:

(I) water analysis chart

METHODOLOGY: the students will prepare a water analysis chart using standard procedures

(Ii) correlation chart

METHODOLOGY: the students will prepare a correlation chart with the standard procedures

(Iii) analysis of published reports

METHODOLOGY: the students will collect and analyze a published report on water quality data

3. **SUB THEME**: water conservation

EXPECTED OUTCOME

The activities will enable the student to

- Understand the different methods of water conservation
- Know about the different techniques for water recycling and recharging

ACTIVITY:

(I) group discussion

METHODOLOGY: the students will discuss in groups to develop strategies for reducing water usage

(Ii) chart/ model preparation/short film/ video clippings

METHODOLOGY: The students will depict the standard procedures for water recycling and harvesting Methods.

(Iii) case study/ interview presentation

METHODOLOGY: the students will discuss the case study on effective rain water harvesting methods adopted by the public

SECTION III: COMMUNITY ENGAGEMENT PROCESS **105 HRS.**

Based on the choice of the sub theme, the students will do the following:

SUB THEMES – WATER POLLUTION AND WATER QUALITY ANALYSIS

To understand the level of pollution in the water bodies and analyze the samples, the following actions shall be
PERFORMED.

- A community with water related problems will be identified with the help of local media, visits, Interaction with the neighbourhood and through other sources.
- Ssurvey on the various water resources of the selected community based on geographic information System (gis).
- Classify their usage as drinking, domestic or agricultural purpose
- Inspect possible sources of pollution
- Collect data through questionnaire from the community to relate health and water pollution
- Compile the information and suggest a suitable experimental analysis to quantify the level of pollution
- Analyze the required water quality parameters using standard procedures
- Compare the analyzed data with the standard water quality parameters
- Suggest suitable methods to mitigate / prevent water pollution in the selected community

SUB THEME - WATER CONSERVATION

- A community with water related problems will be identified with the help of local media, visits, interaction with the neighbourhood and through other sources.
- Survey on the various water resources of the selected community based on geographic information system (gis).
- Study on the various conservation methods adopted by the community and previous history of seasonal rainfalls.
- Collect data on the demand and supply of the water for the selected population.
- Analyze the prevalence and extent of water scarcity.
- Identify possible methods to reduce water scarcity in different seasons (winter/ summer)
- Classify the methods to reduce/recycle and reuse/recharge methods
- Suggest suitable methods or strategies to reduce, reuse and recycle (grey water recycling) and Recharge (rain water harvesting methods) water.

The student will document her engagement with the community through this process in the form of a report with supporting evidences (photographs, video, community feedback etc.). The student will present her outcome of learning process in the form of a oral presentation.

CHE6501CT APPLICATIONS OF CHEMINFORMATICS

(Lab cum Theory)

LEARNING OUTCOME : **4T + 1L Hrs./Wk.**

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

- Identify the lead compounds.
- Describe the various drug receptor interactions.
- Analyse the activity of the drug molecules .
- Evaluate the druglikliness of molecules.

COURSE OUTLINE :

UNIT-I : INTRODUCTION TO DRUG-DESIGN AND DISCOVERY **15T Hrs./Wk.**

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- semi synthesis, improvements in natural products, biosynthetic modification- Structure based drug design-**Case studies**: Anti-influenza drug, HIV protease inhibitors, Fast acting insulin.

UNIT-II : MOLECULAR RECOGNITION IN DRUG-TARGET BINDING **15T Hrs./Wk.**

Thermodynamic considerations, Physical basis of intermolecular interactions – enthalpy, entropy – Total energy of intermolecular interactions – Free energy, Determination of the affinity-Electrostatic interactions, Hydrophobicity, Shape complementarity, Hydrogen bonding interaction, van der waals interactions; **Sterochemistry in drug design**-examples – antihypertensive agent propranolol, therapeutic benefits of quinine and quinidine, cough suppressant dextromethorphan, (-)-dobutamine an antagonist at - adrenoceptors, racemic 3,4-dicarboxypgenylglycine, - arylpropionic acids as nonsteroidal anti-inflammatory drugs.

UNIT-III : MOLECULAR DESCRIPTORS AND STRUCTURE-ACTIVITY RELATIONSHIP **15T Hrs./Wk.**

Introduction, Classification, **Descriptors calculated from 2D structure**-Simple counts, physico-chemical properties, molar refractivity, topological indices, Kappa shape indices, 2D fingerprints, BCUT-**Descriptors based on 3D representations**- 3D fragment screens, pharmacophore keys, **Quantitative structure-activity relationships(QSAR)**(- graphs and equations, physicochemical properties- hydrophobicity, electroeffects, 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- **Statistical analysis**- Linear and Non linear Methods, PLS, PCA, PCR, ANN.

UNIT-IV : DOCKING **15T Hrs./Wk.**

Drug likeliness and compound filters-Prediction of ADME properties-Ligand based Drug Design, Lipinski's rule of five - 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 etc.,. Quantitative Structure Toxicity Relationships (QSTR), Aquatic Toxicity, Carcinogenicity, Mutagenicity

UNIT-V : LAB **15L Hrs./Wk.**

Searching and Retrieving

- molecular data
- physico chemical properties
- biological, toxicological data from web sources for QSAR, QSPR and QSTR related studies. Molecular Property Calculation

Retrieval of protein target

Docking a lead compound into the active site of target

TEXT BOOK(S)

Graham L. Patrick, **An introduction to medicinal chemistry**, 4th: Oxford university press, 2009.
Larsen et al (ed),, **Textbook of Drug Design and Discovery,**, 4th, London and NewYork: Taylor and Francis, 2004.

REFERENCE BOOK(S)

Andrew R. Leach, Valerie J. Gillet, **An Introduction to Chemoinformatics**, revised edition, Springer, Netherland,, 2007..
Ashutosh Kar, **Medicinal Chemistry**, New Delhi, New Age International publishers, 2006..
Ganellin C.R, Roberts S.M,, **Medicinal chemistry, the role of organic chemistry in drug research**, 2nd edition., Elsevier, 1993.
Johann Gasteiger(ed.), Thomas Engel (ed.),, **Chemoinformatics: A Textbook, Wiley VCH,**, Weinheim, 2003..
Leach A.R, **Molecular Modelling: Principles and applications**, 2nd edition, New Delhi, Prentice Hall, 2001.
Patrick G.,, **Instant notes Medicinal chemistry**, Viva books private limited, 2002.

CHE6501CM 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, functional group interconversion - Introduction to disconnection approach - protecting groups.

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, green solvents – water, supercritical CO_2, ionic liquids , solventless reactions, phase transfer catalysts, biocatalysts 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. NMRNuclear 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)

Jag Mohan,,**Organic Spectroscopy**, 2nd, New Delhi: Narosa Publishing House, 2004.

Jain. M. K., Sharma, S. C, **Modern Organic Chemistry**, 4th edition.: Vishal Publishing, New Delhi.

REFERENCE BOOK(S)

Mackie and Smith, **Guide Book to Organic Synthesis**, ELBS, 1982,.

Pavia, Chapman and Kriz, **Introduction to Spectroscopy**, 3rd Edition, Thomson, 2007.

Robert E. Ireland, **Organic Synthesis**, Prentice Hall of India, 1969..

Silverstein, Bassler and Morril, **Spectrometric Identification of Organic Compounds**, , 5th Edition, NewYork, John Wiley and Sons, 1991.

Stuart Warren, **Organic Synthesis, The Disconnection Approach,**, John Wiley & Sons, 2004..

William Kemp,,**Organic Spectroscopy**, 4thEdition., ELBS, 1991,.

WEBSITE(S) :

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

CHE6502CM PHOTOCHEMISTRY, PHASE EQUILIBRIA AND INSTRUMENTAL ANALYSIS (Theory)

LEARNING OUTCOME : **5 Hrs./Wk.**

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

- apply suitable instrumental technique for analysis of chemical compounds.
- describe the various photophysical and photochemical processes.
- illustrate the behavior of chemical mixtures using suitable phase diagrams.
- predict the electric and magnetic properties of molecules.
- explain the properties of polymers.

COURSE OUTLINE :

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 - hydrogen-chloride and hydrogen-bromide - photophysical processes- chemiluminescence – bioluminescence – photosensitization, quenching- applications of photochemistry- laser action.

Concepts for virtual lab:

Photophysical processes.

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-the water, sulfur systems-liquid Helium system - 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 : 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-IV : INSTRUMENTAL METHODS OF ANALYSIS **15 Hrs.**

Principles and method of analysis using optical (Atomic Absorption Spectroscopy, Spectrophotometry, Flame photometry, Fluorimetry, Nephelometry and Turbidimetry) - thermal (Thermo Gravimetric Analysis and Differential Thermal Analysis) and electroanalytical techniques (Amperometry, Coulometry, Voltammetry)

Concepts for virtual lab

Analysis of compounds using different instruments.

UNIT-V : 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 – applications of important polymers-Polyethylene, Polyvinyl chloride, Polystyrene. – Commercially important polymers - Nylon, Teflon

Concepts for virtual lab

Determination of viscosity average weight of polymers.

TEXT BOOK(S)

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

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

Puri.B.R, Sharma.L.R and Pathania.S.,, **Principles of Physical Chemistry**, 46 th: Vishal Publishing Co., Jalandhar,, 2012.

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

CHE 6503CM MOLECULAR SPECTROSCOPY, QUANTUM CHEMISTRY AND GROUP THEORY THEORY

5hrs /Wk

LEARNING OUTCOME:

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.
- recognize the differences between a classical and quantum mechanical systems.
- explain the fundamental principles of quantum mechanics.
- describe the behavior of quantum mechanical systems.
- predict the symmetry elements and point group of a molecule.

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 oscillator-fundamentals, overtones and hot bands-fundamental vibrations and symmetry in polyatomic molecules.

Concepts for virtual lab:

Interaction of EMR with molecules.

Types of rotators.

Fundamental vibrations of a molecule.

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.

Concepts for virtual lab:

Rayleigh and Raman Scattering in molecules.

Franck Condon Principle.

Resonance absorption in spin resonance spectroscopy.

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 and phototelectric effect - operators in quantum mechanics - linear

operator-commutative property – real and imaginary functions and operators - eigenfunctions and eigenvalues.

Concepts for virtual lab:

Wave - particle duality of light and matter.

Black body radiation and photoelectric effect.

UNIT IV: QUANTUM MECHANICS II **15 hrs**

Schrodinger wave equation- characteristics of wave functions- significance of wave functions - particle in 1D and 3D box - allowed energies and degeneracy of energy levels **-** postulates of Quantum mechanics – linear momentum and angular momentum operators – Hermitian operators– orthonormal wave functions - Hamiltonian for the hydrogen and helium atoms.

Concepts for virtual lab:

Wave functions and energy levels of particle in 1D and 3D box.

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 – the Great Orthogonality Theorem - construction of character tables – C_{2V} and C_{2h} point groups.

Concepts for virtual lab:

Symmetry elements and symmetry operations.

TEXTBOOK BOOK(S)

Puri.B.R, Sharma.L.R and Pathania.S., **Principles of Physical Chemistry** , Vishal Publishing Co., Jalandhar, 2012, 46 th edition .

REFERENCE BOOK (S):

Banwell. N & Mc Cash.M., **Fundamentals of Molecular Spectroscopy**, Tata McGraw Hill Publishing Co Ltd. New Delhi, 1994.

Chandra. A.K**., Introductory Quantum Chemistry,** , Tata McGraw Hill Publishing Co. Ltd., New Delhi, 1994, 4th edition.

Ramakrishnan V. and Gopinathan M.S., **Group Theory In Chemistry**, Vishal Publications, 1998.

Raman K.V., **Group Theory and Its Applications to Chemistry**, Tata McGraw-Hill, 1990.

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