

SACRED HEART COLLEGE (AUTONOMOUS)

Tirupattur – 635 601, Tamil Nadu, S.India

Ready for Every Good Work Resi: (04179) 220103College: (04179) 220553Fax: (04179) 226423

A Don Bosco Institution of Higher Education, Founded in 1951 * Affiliated to Thiruvalluvar University, Vellore * Autonomous since 1987

Accredited by NAAC (4th Cycle – under RAF) with CGPA of 3.31 / 4 at 'A+' Grade

B. Sc. CHEMISTRY Program Structure (from 2021 – 2022 onwards)

Year /	Part	Subject	Title of the Paper	Hrs /	Cre	Exam	N	lax Ma	rks
Semester				Week	dits	hours	CIA	Sem	Total
I Year / I Semester	Ι	Tamil	Tamil – I	5	3	3	50	50	100
	II	English	English – I	5	3	3	50	50	100
	II		Communicative English		1				
	III	Core	Organic Chemistry – I	3	3	3	50	50	100
	III	Core	Analytical Chemistry - I	4	4	3	50	50	100
	III	Core Practical	Volumetric Analysis	3	3				
	III	Allied	Allied Mathematics – I	6	4	3	50	50	100
	IV		FC	2	1				
	IV		Religion & Ethics – I	2	1	3	50	50	100
	Ι	Tamil	Tamil – II	5	3	3	50	50	100
	II	English	English – II	5	3	3	50	50	100
	II		Communicative English		1				
I Year /	III	Core	Inorganic Chemistry - I	3	3	3	50	50	100
I I Cal / II	III	Core	Physical Chemistry – I	4	4	3	50	50	100
Semester	III	Core Practical	Volumetric Analysis	3	3	3	50	50	100
	III	Allied	Allied mathematics - II	6	4	3	50	50	100
	IV		FC	2	1	3	50	50	100
	IV		Religion & Ethics – II	2	1	3	50	50	100
	Ι	Tamil	Tamil – III	5	3	3	50	50	100
	II	English	General English – III	5	3	3	50	50	100
	III	Core	Organic Chemistry – II	3	3	3	50	50	100
II Year / III Semester	III	Core	Inorganic Chemistry – II	4	4	3	50	50	100
	III	Core	Qualitative Inorganic	3	3				
	TTT	Practical	Analysis	(4	2	50	50	100
	III IV	Allied	Allied Physics – I FC	6 2	4	3	50	50	100
	IV		Human Rights	2		3	50	50	100
	V		DEEDS	Ĺ	1	3	50	50	100
	V V		SHELTERS						
	v		Certificate course – I		2*				
II Year /	Ι	Tamil	Tamil – IV	5	3	3	50	50	100
11 1 Cal /	1		1 uilii — 1 v	5	5	5	50	50	100

IV	II	English	English – IV	5	3	3	50	50	100
Semester	III	Core	Organic Chemistry - III	3	3	3	50	50	100
	III	Core	Physical Chemistry - II	4	4	3	50	50	100
	III	Core Practical	Qualitative Analysis	3	3	4.5	50	50	100

Year /	Par	a 11 (Hrs /	Cre	Exam	Max Marks		
Semester	t	Subject	Title of the Paper	Week	dits	hours	CIA	Sem	Total
	III	Allied	Allied Physics – II	6	4	3	50	50	100
II Year /	IV		FC	2	1		50	50	100
IV	IV		Environmental Studies	2	1	3	50	50	100
Semester	V		DEEDS		2				
	V		SHELTERS		2				
	III	Core	Organic Chemistry – IV	4	4	3	50	50	100
	III	Core	Inorganic Chemistry – III	4	4	3	50	50	100
	III	Core	Physical Chemistry – III	4	4	3	50	50	100
	III	Core	Analytical Chemistry –II	4	4	3	50	50	100
	III	Main Elective	Elective – I	3	2	3	50	50	100
III Year /	III	Main Elective	Elective – II	3	2	3	50	50	100
V Semester		SSP	Chemistry for Competitive Exam – I		1*				
	III	Core Practical	Gravimetric & Organic Analysis	3	3		50	50	100
	III	Core Practical	Physical Chemistry Practicals	3	3		50	50	100
		NME	Chemistry of Drugs and Disease	2	1		50	50	100
			Certificate Course - II		2*				
	III	Core	Organic Chemistry – V	4	4	3	50	50	100
	III	Core	Inorganic Chemistry – IV	4	4	3	50	50	100
	III	Core	Physical Chemistry – IV	4	4	3	50	50	100
	III	Subject Skill (SS-I)	Paper – I	5	4	3	50	50	100
III Year /	III	Subject Skill (SS-II)	Paper – II	5	4	3	50	50	100
VI Semester	IV	NME	Chemistry in Everyday Life	2	1	3	50	50	100
	III	SSP	Chemistry for Competitive Exam – II		1*				
	III	Core Practical	Gravimetric & Organic Analysis	3	3	6	50	50	100
	III	Core Practical	Physical Chemistry Practicals	3	3	3	50	50	100
			Internship/Iindusdrial Visit/ Case study/Project*		2*				
	tua au		Total	180	148 +2* +2* +2*				

* Extra credits

Note:

FC

 $SSP/Project/Certificate\ course-optional$

Abbreviations

Foundation Course

SEM I CH116 Organic Chemistry – I Hrs/week – 3 hours (Credits 3) **Objectives**

- Understanding the structure of organic compounds. •
- Understanding the fundamentals of acidity and basicity. •
- Providing the rudimentaries of stereochemistry.

Unit 1 Electronic structure and bonding

- 1.1 Ionic and covalent bonds, Polar covalent bonds and dipole moment. Introduction to molecular orbital theory, Single, double, and triple bond formation in organic compounds.
- 1.2 Bonds in methyl cation, radical and anion. Bonds in water, ammonia, ammonium ion and hydrogen halides. Hybridization, bond lengths, strengths, and angles. Fischer, Flying wedge, Newmann projection and Sawhorse representations .Rotation about carbon-carbon single bonds, conformational analysis of ethane, butane.
- 1.3 Baeyer strain theory-conformational analysis of cyclohexane

Unit 2 Acidity and basicity of organic compounds

- 2.1 Acids and Bases, pKa and pH, organic acids and bases, Acid-base reaction and position of equilibrium, Effect of structure on the pKa of acids(electronegativity, hybridization, size).
- 2.2 Effect of substituent on the strength of an acid, delocalized electrons. Buffer solutions, Lewis acids and bases.
- 2.3 Effect of pH on the structure of organic compounds.

Unit 3 Stereochemistry 1

- 3.1 Isomerism, constitutional, conformational isomers, stereoisomers, cis-trans isomers from restricted rotation, asymmetric centers and stereocenters.
- 3.2 Isomers with one and two asymmetric centers, configurational isomers, Cahn Ingold Prelog rules and assigning E, Z, R & S to molecules.
- 3.3 Optical activity, measurement of specific rotation, enantiomeric excess, meso compounds with an asymmetric center, reactions of compounds that contain an asymmetric center-Stereoselective, regioselective and stereospecific reactions.

Unit 4 Chemistry of Alkenes

- 4.1 Stereochemistry of electrophilic addition reactions of alkenes. Addition reactions resulting in one and two asymmetric centers: addition reactions forming a cyclic bromonium ion intermediate.
- 4.2 Alkenes, addition of hydrogen halides, stability of carbocations, electrophilic addition reactions and regioselectivity.
- 4.3 Addition of water, alcohols, halogens, peroxy acid and hydrogenation of alkenes. Oxymercuration-reduction and hydroboration-oxidation with mechanism.

Unit 5 Chemistry of Alkynes

- 5.1 Alkynes: Structure and reactivity of alkynes(with mechanism).
- 5.2 Addition of hydrogen halides, halogens, water, hydroboration-oxidation
- 5.3 Addition of hydrogen to an alkyne, acidity of hydrogen bonded to an 'sp' carbon, synthesis using

9 Hours

9 Hours

NAAC 5th CYCLE

9 Hours

9 Hours



Reference Books:

Text Book

1. Paula Yurkanis Bruice, Organic chemistry, 6th Edition, Prentice Hall, Illinois, 2011.

Further reading

- 2. R.T. Morrison and R. N. Boyd, *Organic chemistry*, 6th Edition, Prentice-Hall of India, New Delhi, 2008.
- 3. Leroy. G. Wade, *Organic chemistry*, 6th Edition, Pearson, New York, 2005.
- 4. Clayden, J Greeves, N and Warren, S, *Organic Chemistry*, 2nd Edition, Oxford University Press, New York, 2001.
- 5. Loudon, Marc G, Organic Chemistry, 6th Edition,. Oxford University Press, New York, 2016.

Outcomes

- Ability to draw the structure of molecules.
- Assess the acidic, basic and delocalization nature of molecules.

SEM I CH117-Analytical Chemistry – I Hrs/week – 4 (Credits 4) Objectives

- To learn the basic principles and applications of important analytical techniques
- To develop a sound knowledge in chemistry involved in an analysis

Unit-1. Laboratory hygiene and Safety

- 1.1. Storage and handling of corrosive, flammable, toxic, carcinogenic and poisonous chemicals. Disposal of solid, liquid and fume wastes.
- 1.2. Simple First Aid Procedures: Acids, alkalis, phenols, toxic substances like bromine, benzene, pyridine, glass cuts and poisons. Universal antitodes, tartaremetic and tincture of iodine.
- 1.3 Laboratory Glassware-Cleansing agents-interchangeable ground joints apparatusdescription, advantages and precautions to be followed. Safety practices in the laboratory.

Unit - II Separation Techniques

- 2.1 Solvent Extraction-Principle-Extracting from solid-liquid phases-Soxhlet extractor Extraction by chemically active Solvents-Chromatography-types of chromatography.
- 2.2 Principle, techniques and applications of TLC, and Paper. Principle, techniques and applications of Column chromatography.
- 2.3 Gas-Liquid Chromatography-Principle, Instrumentation, and applications.

Unit-III Volumetric analysis

- 3.1 Primary and secondary standards. Requirements of primary standards with examplesclassifications of volumetric analysis. Acid-base titrations: Principle-theory of acidbase indicators- Methyl red and phenolphthalein.
- 3.2 Redox titrations: Theory of redox titrations-theory of redox Indicators-Diphenyl amine, Ferroin, and Starch.
- 3.3 Precipitation Titrations: Principle-Estimations of Chloride by Mohr's method and Volhard's Method. Complexometric Titrations: Principle-Estimation of Magnesium using EDTA-Theory of metal-ion indicators.

Unit - IV Gravimetric Analysis and Thermal Analysis

12 Hours

12 Hours

12 Hours

CRITERION I

- 4.1 Gravimetric Analysis-Principle-Conditions of precipitation-choice of Precipitants. Inorganic and Organic Precipitants-specific and selective precipitants.
- 4.2 Masking Agents-Precipitation from homogeneous Medium-Post Precipitation-Co-Precipitation-Differences between post and Co-precipitation.
- 4.3 Principles of thermogravimetric analysis and Instrumentation-Derivative thermogravimetry-Factors influencing thermogram. DTA-Principle and Instrumentation-Applications: TGA-Calcium oxalate monohydrate-DTA-Calcium acetate monohydrate.

Unit - V Units of measurement and Error Analysis

12 Hours

- 5.1 Units of measurement-normality, molality, and molarity, examples for this concept. Mole fraction-percentage solution
- 5.2 Significant Figures-Rules-Rounding off figures. Definition of terms in mean, median, and mode. Standard deviation, relative standard deviation.
- 5.3 Precision and Accuracy-absolute error, relative error. Types of error in experimental data, determinate (systematic), indeterminate (or random) and gross.

References

- 1. Gary D. Christian,; Purnendu K. Dasgupta,; Kevin A. Schug, *Analytical Chemistry*, 7thEdition;Wiley Global Education, 2013.
- 2. Douglas A. Skoog,; F. James Holler,; Stanley R. Crouch, *Principles of Instrumental Analysis*, 6thEdition;Cengage Learning, 2006.
- 3. John H Kennedy, *Analytical Chemistry: Principles*, 2ndEdition; Saunders College Pub, 1990.
- 4. Larry G. Hargis, *Analytical Chemistry: Principles and Techniques*, 1stEdition; Prentice Hall, 1988.
- 5. Reuben Alexander Day,; Arthur Louis Underwood, *Quantitative Analysis*, 6thEdition;Prentice Hall India Learning Private Limited, 1992.
- 6. S. M. Khopkar, *Basic Concepts of Analytical Chemistry*, 3rd Rev Edition; New Age Science Ltd, 2008.
- 7. Frank A. Settle, *Handbook of Instrumental Techniques for Analytical Chemistry*, 1stEdition; Prentice Hall, 1997.
- 8. R.Gopalan, P. S. Subramanian and K. Rengarajan, *Elements of analytical chemistry*, 3rdEdition, Sultan Chand, New Delhi, 2003
- 9. A. K. Srivatsava and P. C. Jain, *Chemical Analysis and Instrumental Approach*, 3rdEdition, S.Chand and Company Ltd., New Delhi, 2010.

Learning Outcomes

- Identify the suitable methods for separation; explain chemical analysis of compounds
- Outline the principle behind Volumetric, gravimetric analysis, mass spectrometry, Chromatography and list out their applications

SEM II CH216-Inorganic Chemistry - I **Objectives**

- To understand the basic atomic structure of elements their periodic properties and chemical bonding.
- To learn the properties and applications of *s* and *p* block elements.
- To understand the principles and theories of Acids and Bases

Unit-1 Atomic Structure

- 1.1 Electronic configurations of the elements, Aufbau principle, quantum numbers, and Pauli's exclusion principle. Hund's multiplicity rule for filling electrons in various orbitals, Stability of half-filled and completely filled orbitals, effective nuclear charge.
- 1.2 Shapes of s, p, d orbitals s, p, d and f block elements classification and characteristic properties.
- 1.3 Periodicity of properties Definition and periodicity of the following properties Atomic radii - factors affecting atomic radii - ionic radii - factors affecting ionic radii. Ionisation potential - factors affecting ionisation potential - Electron affinity factors affecting electron affinity - Electronegativity - factors affecting electronegativity – Pauling scale.

Unit-2 Chemical Bonding

- 2.1. Ionic Bonding: General characteristics of ionic bonding. Energy considerations in ionic bonding, lattice energy and solvation energy and their importance in the context of stability and solubility of ionic compounds. Statement of Born-Landé equation for calculation of lattice energy, Born-Haber cycle and its applications.
- 2.2 Polarizing power and polarizability. Fajan's rules, ionic character in covalent compounds, bond moment, dipole moment and percentage ionic character.
- 2.3. Covalent bonding: Lewis theory, Octet theory, VSEPR theory and applications geometries of BCl₃, H₂O, ClF₃, PCl₅, IF₇ and XeF₆ molecules.

Unit-3 Alkali and alkaline earth metals

- 3.1 Alkali metals Comparative study of elements oxides, halides, hydroxides and carbonates – Exceptional property of Lithium – Diagonal relationship of Li with Mg.
- 3.2. Alkaline earth metals comparative study of the elements with respect to oxides, hydroxides, halides, sulphates and carbonates – Exceptional property of Beryllium – Diagonal relationship of Be with Al
- 3.3. Comparison of alkaline earth metals with alkali metals Magnesium acting as bridge element between IIA and IIB groups - Magnesium resembles zinc.Properties and uses of Alkaline earth metals. Biological role of Mg²⁺ and Ca²⁺

Unit-4 p-block elements, Chemistry of group 13

- 4.1. Main group elements- introduction, general and special characteristics. Group 13: general properties, electronic configuration, oxidation states, inert pair effect, size of atoms and ions, electropositive nature and ionization energy.
- 4.2 Compounds of group 13: Structure and bonding in diborane. Preparation, properties and structure: Borazine, trihalides- Boron and Aluminium.
- 4.3 Compounds of Boron and Oxygen (structure and properties): Sesquioxides-Borates and Borax.

Unit-5 Acids and Bases

9 Hours

Hrs/week – 3 (Credits 3)

9 Hours

9 Hours

9 Hours

- 5.1. Arrhenius concept. Lowry Bronsted concept-conjugate acid-base pairs, relative strengths of acid-base pairs.
- 5.2. Lux-flood concept. Lewis concept, limitations of lewis concept.
- 5.3. Pearson concept-HSAB principle.Estimation of TDS in water.

Learning Outcomes

- The student can explain the atomic structure and bonding nature present in a molecule along with the applications and importance of s and p block elements
- \succ The students can understand the theories pertaining to the acids and bases.

References

- 1. R. D. Madan, *Modern Inorganic Chemistry*, Second edition, S. Chand publications, New Delhi, 2000.
- 2. B. R. Puri, L. R. Sharma and K. C. Kalia, *Principles of Inorganic Chemistry*, 33rd Edition, Vishal Publishing Co, Jalandar, 2004.

(Advanced Reading)

- 1. C. Chambers and A. K. Holliday, *Modern Inorganic Chemistry*, First edition, Butterworth and Co., Sussex, 1975.
- 2. Gary L Miessler and Donald A Tarr, *Inorganic Chemistry*, Third edition, Pearson Prentice Hall.
- 3. B. Murphy, C. Murphy and B. J. Hathway, *Basic Principles of Inorganic Chemistry*, The Royal Society of Chemistry, Cambridge, 1998.

SEM II CH217-Physical Chemistry - I

Hrs/week – 4 (Credits 4)

Objectives

- To understand the important behaviour of gases and liquids
- To learn the fundamentals of thermochemistry and thermodynamics

Unit – I Gaseous State -I

- 1.1. Kinetic theory of gases –derivation of kinetic gas equation–Gas laws from the kinetic gas equation.
- 1.2. Maxwell's distribution of-molecular velocities (no derivation)–Experimental verification of velocity distribution Effect of temperature on velocity distribution.
- 1.3. Kinds of velocities mean, rms, most probable velocities-Degrees of freedom of a gaseous molecule, equipartition of energy, heat capacity on molecular basis.
- 1.4. Collision diameter-Collision Number-Collision frequency-and mean free path

Unit - II Gaseous State -II

2.1 Effect of Temperature and Pressure on mean free path and Collision frequency

- 2.2 ideal gas and real gas-Deviation of real gas from ideal behaviour-Compressibility factorcauses of deviation-Compressibility of various Gases (variation of Z with Pressure)
- 2.3 Derivation of van der Waals Equation for real gases-significance of van der Waals constants-Behaviour of real gas using van der Waals equation-Exceptional behaviou of H and He.

2.4 Liquification of gases-Linde'sProcess and Claudes Process

Unit -III Liquid State

12 Hours

12 Hours

- liquids –Vapour pressure and Factors affecting them Determination of Vapour pressure of a liquid -3.2 Surface tension of a liquid-surface energy-liquid raises in a capillary tube-surface active
 - 3.2 Surface tension of a liquid-surface energy-liquid raises in a capillary tube-surface active agents Effect of temperature on surface tension-Determination of surface tension-

Differences between solids/liquids/gases in terms of structure-Intermolecular forces in

- 3.3 Capillary Rise and Drop Weight Method-Drop weight methods
- 3.4 Viscosity-factors affecting viscosity-Ostwald Viscometer method

Unit-IV: Thermodynamics -I

3.1

12 Hours

- 4.1. Thermodynamics Definition and explanation of terms System, boundary, surroundings Homogeneous and heterogeneous system Isolated system Closed system Open system. Thermodynamic functions Intensive and extensive properties state functions and path functions. Exact differentials
- 4.2. Thermodynamic processes First law of thermodynamics Concept of internal energy Energy changes with work –State functions.
- 4.3. Enthalpy (Heat) of the reaction- Factors influencing enthalpy-Measuring the enthalpy of combustion (Bomb Calorimeter)
- 4.4 Heat capacity at constant pressure and volume relationship between Cp and Cv

Unit-V: Thermochemistry

12 Hours

- 5.1 Joule's law Joule Thomson effect Joule Thomson coefficient and its derivation inversion temperature, its significance and its derivation.
- 5.2 Endothermic/Exothermic reaction. Enthalpy of formation and standard enthalpy of formation-importance of standard enthalpy of formation- Hess'a Law of constant heat summation
- 5.3 Determination of enthalpy of formation Problems related to Hess's Law Bond enthalpy and application -calculation from thermochemical data
- 5.4 Application of bond dissociation energies calculation from thermochemical data Kirchoff's equation and its significance.

Text Books:

- 1. B. R. Puri, L. R. Sharma and M. S. Pathania, *Principles of Physical Chemistry*, 47th Edition, Vishal Publishing Co, Jalandar, 2016.
- 2. R.L. Madan, *Physical Chemistry*, Mc Graw Hill Education Pvt. Ltd. 2015.
- 3. Peter Atkins and Julio de Paula, *Physical Chemistry*, 10th Edition, W. H. Freeman and Company. (Unit IV)
- 4. Raymond Chang and John W. Thoman, *Physical Chemistry for the chemical science*, Jr.University Science Books (Unit IV)

Reference:

- 1. Arun Bahl, B.S. Bahl. G.D.Tuli, Essentials of Physical Chemistry, S. Chand Publications
- 2. A.S. Negi and S.C. Anand, A text book of Physical Chemistry, Wiley Eastern Ltd, New Delhi, 1984.

Learning Outcome:

- Recognize and relate the properties of ideal and real gases
- Describe the properties of liquids
- Describe the thermodynamic parameters in exo and endothermic process.

Semester - I & II PCH209-Volumetric Analysis 3 Hrs/week (3 Credits/ semester)

Objectives

- To learn the methods to estimate chemical substances through various volumetric procedures
- To appreciate the merits and limitations of each type of analysis and acquiring knowledge about the implementation of these procedures for specific ions/species.

Acidimetry

- 1. Estimation of Borax Standard Sodium Carbonate
- 2. Estimation of Sodium Hydroxide Standard Sodium Carbonate
- 3. Estimation of HCl Standard oxalic acid.

Permanganometry

- 4. Estimation of oxalic acid Standard FAS
- 5. Estimation of FeSO₄– Standard Oxalic acid

Dichrometry

- 6. Estimation of Ferrous Iron using Diphenyl amine as indicator.
- 7. Estimation of ferric ion using Diphenyl amine as indicator

Iodimetry

8. Estimation of Arsenious oxide

Iodometry

9. Estimation of Copper - Standard Potassium dichromate

Complexometry

- 10. Estimation of Magnesium using EDTA
- 11. Estimation of Zinc using EDTA
- 12. Estimation of Calcium using EDTA
- 13. Estimation of total hardness of water.

Cerimetry

14. Estimation of sodium nitrite.

References

- 1. V. Venkateswaran, R. Veerasamy, A.R. Kulandaisamy, *Basic principles of Practical Chemistry*, S.Chand publications, New Delhi, 2002.
- 2. A.O, Thomas. Practical Chemistry, 6th Revised Edition, Sharada Press, 1995.
- 3. J. N. Gurtu and R. Kapoor, *Advanced Experimental Chemistry*, Vol. I –III, S. Chand and Co., 1987.

Semester - I ACH110 Allied Chemistry - I (Biochemistry) 4 Hrs/week (2Credits) **Objectives**

- To understand the basics of chemistry.
- To learn the role of chemistry in biochemistry

Unit - I: Introduction to Solutions-

- 1.1 Units of measurement-normality, molality, and molarity, examples for this concept. Mole fraction-percentage solution.
- 1.2 Significant figures-Rules-Rounding off figures-Errors-types of errors and rectification of errors.
- 1.3 Solutions-solute-solvent(polar and non-polar)-ideal- non ideal solutions with one example each. Raoult's Law Deviations. Isotonic solution, hypertonic solution and hypotonic solution
- 1.4 Water-Structure of Water-weak interactions of water-Water as a reagent.

Unit - II: Basic Organic Chemistry

- 2.1 Structure of Atom-types of Bonds-Valance of carbon-Bond length and bond energies.
- 2.2 Electronic configuration-Hybidisation, sp³, sp², sp Hybridisation of Hetero atoms
- 2.3 Stereo isomerism-types causes of optical activity, optical isomerism of lactic acid and tartaric acid-Racemisation-Resolution-Geometrical isomerism-maleic and fumaric acid.
- 2.4 Concept of resonance-Aomaticity in benzene-Huckle's rule-reactions in benzene(Electrophilic substitution reaction, Addition)

Unit - III: Acid-Base Theory and Buffers in Body Fluid System **12 Hours**

- 3.1 Acids and bases, Arrhenius, Lowry Bronsted concept, Lewis concept-conjugated pairs. pH, pOH, buffer, buffering capacity, common ion effect and Henderson Hesselbalch equation. Buffers in body fluids, red blood cells and tissues.
- 3.2 Colloids: Types of colloids-lyophilic and lyophobic colloids-Tyndell effect, Brownian movement, Protective colloids-Gold number, coagulation of colloids,
- 3.3 Emulsions-type of emulsions, Gels-types of gels, properties of gels.
- 3.4 Osmosis and its applications and osmotic pressure. Principle of sonication, dialysis and Ultra filtration. Isotonic, Hypotonic and hypertonic Solutions.

Unit - IV: Chemical Kinetics

- 4.1 Kinetics: Rate-Rate equation-order-Molecularity-pseudo first order reaction- First order reaction-Pseudo first order (with examples)- derivation of equation for rate constant, determination of order (half-life method, graphical method).
- 4.2 Factors affecting the reaction rate(pressure, temperature, concentration, solvent and catalyst), Energy of activation.
- 4.3 Catalyst: Characteristics of catalyst auto catalyst, enzyme catalyst, active center, catalytic poison, promoters (Definitions of these terms with examples only). Homogenous and heterogeneous catalyst-mechanism of heterogeneous catalyst.
- 4.4 Enzyme catalysis- Theory-Lock and Key Model-Induced Fit Model-Michealis-menton equation-Industrial applications of catalysts.

Unit -V: Anesthetics and Antibiotics

- 5.1 Sulpha Drugs-Introduction-Preparation, uses and mode of action of sulpha drugs. Prontosil, Sulphanilamide, Sulphapyridine, Sulphadiazine, and Sulphaguanidine
- 5.2 Structure and uses of the following antibiotics-Penicillin, chloramphenicaol, and streptomycin.
- 5.3 Anesthetics: Classification of anesthetics with examples(Types of Classifications).

12 Hours

12 Hours

12 Hours

5.4 Preparation, advantages and disadvantages of the following anesthetics- 1) Diethyl ether, 2) Chloroform, 3) Tri chloroethane, and 4) Thiopental sodium

References

- 1. R. D. Madan, *Modern Inorganic Chemistry*, Second edition, S. Chand publications, New Delhi, 2000.
- 2. B. R. Puri, L. R. Sharma and K. C. Kalia, *Principles of Inorganic Chemistry*, 33rd Edition, Vishal Publishing Co, Jalandar, 2004.
- 3. Jayashree Ghosh, *Textbook of Pharmaceutical chemistry*, Rajendra ravindra printers Pvt. Ltd., New Delhi, 2010
- 4. Nelson, D. L.; Cox, M. M.; *Leninger's Principles of Biochemistry*, W H Freeman & Co, 2012.
- 5. R.T. Morrison and R. N. Boyd, *Organic chemistry*, 6th edition, Prentice-Hall of India, New Delhi, 2004.
- 6. Paula Yurkanis Bruice, *Organic chemistry*, 6th edition, Pearson Edition, New York, 2006.

Semester - II ACH210 Allied Chemistry - II (Biochemistry) 4 Hrs/week (2Credits) Objectives

- To understand the basics of chemistry.
- To learn the role of chemistry in biochemistry

Unit - I: Chromatography and Electrophoresis Technique

- 1.1 Principle, Procedure and application of Paper chromatography, partition chromatography.
- 1.2 Principle, Procedure and application of Ion exchange and gel chromatography, partition chromatography.
- 1.3 Principle, Procedure and application of GLC and HPLC.
- 1.4 Electrophoresis:Principle, procedure and application of Free flow and Zone electrophoresis.

Unit - II: Nuclear Chemistry in Biochemistry

- 2.1 Radioactivity-types of rays-natural and artificial radioactivity
- 2.2 Radioactive disintegration-half life-average life- transmutation of elements-group displacement law-Applications of radioactivity.
- 2.3 Isotopes-important stable isotopes used in biochemistry(Medicinal applications of Isotopes)-Radiation hazards and handling the isotopes.
- 2.4 Measurement of radioactivity GM Counter and Scintillation counter

Unit - III: Carbohydrates

- 3.1 Fischer's Projection-Classification and nomenclature of carbohydrates -Stereochemistry of monosaccharides-Configuration of glucose-Anomers-mutarotation.
- 3.2 Reactions and characteristics of aldehyde and keto group, action of acids and alkalies on sugars, reactions of sugars due to hydroxyl group.
- 3.3 Properties of glucose-An introduction to mucopoly saccharides (proteoglycon).
- 3.4 Structure and reaction of mono and disaccharides: glucose, fructose, sucrose, maltose lactose, starch, cellulose and glycogen (No elucidation).

Unit - IV: Amino Acids, Peptides and Proteins

4.1 Classification of amino acids- neutral, acidic, basic, essential and non-essential-Properties of glycine (Physical and chemical).

12 Hours

12 Hours

12 Hours

- 4.2 Peptides- N-terminal and C-terminal residues-nomenclature-End group analysis-Reduction method-Sangers method.
- 4.3 Proteins-classification based on composition, functions, shape and solubility-Primary, Secondary, Tertiary, and quaternary-structure of proteins-Ramachandran Plot.
- 4.4 Denaturation, renaturation and folding of proteins.

Unit -V: Coordination and Bioinorganic Chemistry

12 Hours

- 5.1 Coordination chemistry- Nomenclature- Werner's theory- bonding nature- EAN rule
- 5.2 Valence bond theory, Crystal field theory- tetrahedral, octahedral, square planar complexes and colour of the complexes.
- 5.3 Isomerism in coordination compounds- Ionization, hydrate, linkage, coordination and coordination position isomerism.
- 5.4 Introduction to porphyrin ring systems-Structure and functions of haemoglobin and Chlorophyll.

References

- 1. I. L. Finar, Organic Chemistry Vol I & II, Pearson Education, New Delhi, 2002.
- 2. O. P. Agarwal, Organic Chemistry of Natural Products Vol I & II, Goel Publishing House, New Delhi, 2002.
- 3. Nelson, D. L.; Cox, M. M.; *Leninger's Principles of Biochemistry*, W H Freeman & Co, 2012.
- 4. J.L. Jain,; J. Sunjay,; J. Nithin, *Fundamentals of Biochemistry*, S.Chand Publications, New Delhi, 2004

Semester - III & IV PACH209/PACH409Allied Chemistry Lab Work (Mathematics, Physics and Biochemistry,)2 Hrs / week (4 Credits)

Objectives

- To learn the basics of analysis involved in estimating the amount of substances.
- To acquire the practical knowledge about the analysis of organic compounds

Volumetric Analysis

Estimation of Hydrochloric acid using std. Oxalic acid. Estimation of NaOH using std. Na_2CO_3 Estimation of FeSO₄ using std. FAS solution Estimation of Oxalic acid using std. FAS. Estimation of Fe²⁺ using diphenylamine as indicator.

Qualitative Organic Analysis

Systematicanalysis of organic compounds containing one functional group and characterization by confirmatory tests - Aromatic aldehydes, ketones, carbohydrate, Aromatic carboxylic acid, phenol, aromatic primary amineand amides

References

- 1. V. Venkateswaran, R. Veerasamy, A.R. Kulandaisamy, *Basic principles of Practical Chemistry*, S.Chand publications, New Delhi, 2002.
- 2. A.O, Thomas. *Practical Chemistry*, 6th Revised Edition, Sharada Press, 1995
- J. N. Gurtu And R. Kapoor, Advanced Experimental Chemistry, Vol. I Physical Chemistry, Vol. II Inorganic Chemistry, Vol. III Organic Chemistry, Organic Reactions & Reagents [B.Sc., (Hons.)& M.Sc.], Himalayan Publishers, 1974.

SEM III CH316-Organic Chemistry - II Hrs/week – 3 (Credits 3)

Objectives

- Understanding substitution and elimination reactions.
- Understanding metal carbon bonds.

Unit 1 Delocalisation

- 1.1 Delocalised electrons and benzene's structure, bonding in benzene, reasonance contributors and reasonance hybrids, stability of reasonance contributors, delocalization energy, delocalized electrons and stability, stability of allylic and benzylic cations., molecular orbital description of stability(1,3 Butadiene and 1,4 Penta diene)
- 1.2 Effect of delocalized electrons on pKa values and product of a reaction
- 1.3 Reactions of isolated dienes and conjugated dienes, thermodynamic versus kinetic control of reactions, Diels- alder reaction 1,4 addition, conformations of the diene.

Unit 2 Substitution reactions

- 2.1 Alkyl halides- substitution reactions- S_N2, factors affecting S_N2, reversibility of S_N2 reaction.
- 2.2 S_N1 , factors affecting S_N1 , stereochemistry of S_N1 and S_N2
- 2.3 Competition between S_N1 and S_N2, role of solvents S_N1 and S_N2-Intermolecular versus intramolecular reactions.

Unit 3 Elimination reactions

- 3.1 Elimination reactions, E2 reaction regioselectivity. E1 reaction, competition between E2 and E1 reactions.
- 3.2 E2 and E1 reactions stereo selectivity, elimination from substituted cyclohexanes.
- 3.3 Kinetic isotope effect in mechanism determination, competition between substitution and elimination.

Unit 4 Alcohols and Amines

- 4.1 Conversion of alcohols to alkyl halides, alcohols to sulfonate esters, elimination reactions of water from alcohols, oxidation of alcohols.
- 4.2 Nucleophilic substitution reaction of ethers, epoxides.
- 4.3 Substitution or elimination reactions in amines, Elimination reactions of quaternary ammonium hydroxides, phase transfer catalysis(concept only). Reactions of thiols, sulfides and sulfonium salts.

Unit 5 Organometallic compounds

- 5.1 Metal carbon bond, Synthesis of Grignard reagents and Organolithium compounds.
- 5.2 Organo metallics by deprotonating alkynes, Ortholithiation. Primary, secondary and tertiary alcohols from aldehydes and ketones.
- 5.3 Reactions of organolithium and Grignard reagents with electrophiles, transmetallation, coupling reactions, palladium catalyzed coupling reactions, alkene metathesis.

Reference Books:

Text Book

1. Paula Yurkanis Bruice, Organic chemistry, 6th Edition, Prentice Hall, Illinois, 2011.

9 hours

9 hours

9 hours

9 hours

Further reading

- 2. R.T. Morrison and R. N. Boyd, Organic chemistry, 6th Edition, Prentice-Hall of India, New Delhi, 2008.
- 3. Leroy. G. Wade, *Organic chemistry*, 6th Edition, Pearson, New York, 2005.
- 4. Clayden, J Greeves, N and Warren, S, Organic Chemistry, 2nd Edition, Oxford University Press, New York, 2001.
- 5. Loudon, Marc G, Organic Chemistry, 6th Edition, Oxford University Press, New York, 2016.

Outcomes

- Ability to differentiate elimination and substitution reactions.
- Knowledge on application of intermediates and mechanism.
- Knowledge on the synthetic nature of organometallic compounds.

SEM III CH317-Inorganic Chemistry - II Hrs/week – 4 (Credits 4) **Objectives**

- To have a sound knowledge about structure and shape using VB and MO theory
- To know about Chemistry of group-14 and 15 and its applications
- To understand the importance of Nuclear chemistry and its applications

Unit-1 VB and MO Theory

- 1.1 Valence bond theory postulates and limitations hybridization explanation with examples.
- 1.2 Concept of resonance and resonating structures in various inorganic and organic compounds. MO Approach: Rules for the LCAO method, bonding and antibonding MOs.
- 1.3 MO treatment of homonuclear diatomic molecules: H₂, N₂, O₂, and F₂. Heteronuclear diatomic molecules: HF, CO, and NO
- 1.4 Comparison of VB and MO approaches.

Unit-2 Chemistry of Group 14

- 2.1 Group 14: general properties, electronic configuration, metallic character, and oxidation states.
- 2.2 Uniqueness of Carbon and Silicon in comparison to remaining elements. Carbides-Preparation, classification and applications. Allotropes of Carbon- structure, properties and uses. Oxides of carbon (structure and properties):
- 2.3 CO, CO₂ and carbon suboxides. Carbon cycle.
- 2.4 Silicates-classification, properties, structure and uses. Silicones- Polysiloxanes.

Unit-3 Chemistry of Group 15

- 3.1 Group 15: general properties, electronic configuration, oxidation states.
- 3.2 Compounds of group 15: Hydrides of Nitrogen and Phosphorus, Haber's process, Oxides of Nitrogen: NO, NO₂, N₂O, and N₂O₃ (structure, properties and uses).
- 3.3 Oxo-acids of Nitrogen and Phosphorous- preparation and structure.
- 3.4 Polyphosphates-preparation and structure.

Unit-4 Nuclear Chemistry

- 4.1 Fundamental particles of the nucleus- nucleon, nuclides, isotopes, isobars, isotones.
- 4.2 Nuclear radius, nuclear mass, nuclear density, nuclear forces operating between the nucleons, and packing fraction.

12 hours

CRITERION I

12 hours

12 hours

- 4.3 Natural radioactivity- nuclear reactions, radioactive decay, group displacement law, N/P ratio, curves, stability belts and rate of radioactive disintegration.
- 4.4 Nuclear binding energy. Mass defect, simple calculations involving mass defect and B.E per nucleon, Q value determination, magic numbers.

Unit-5 Applications of Nuclear Chemistry

- 5.1 Detection and measurement of radioactivity- G. M counter, and scintillation counter. Application of radioisotopes as tracers: Rock and Carbon dating.
- 5.2 Artificial radioactivity: artificial transmutation of elements and Particle acceleratorscyclotron. Induced radioactivity and preparation of transuranic elements.
- 5.3 Nuclear fusion reactions and applications: nuclear fusion in the sun and hydrogen bomb. Safe disposal of radioactive waste.
- 5.4 Preparation of Inorganic Complexes (Any two)

Learning Outcome:

- > The student will understand the chemistry of 14 and 15 group.
- > The student can know the importance of nuclear chemistry and its applications
- The student can understand the structure and shape of the molecule using VB and MO theory.

References

(Text Book)

- 1. R. D. Madan, *Modern Inorganic Chemistry*, Second edition, S. Chand publications, New Delhi, 2000.
- 2. B. R. Puri, L. R. Sharma and K. C. Kalia, *Principles of Inorganic Chemistry*, 33rd Edition, Vishal Publishing Co, Jalandar, 2004.
- 3. H. J. Arnikar, *Essentials of nuclear chemistry*, Fourth Edition, New Age International Private Limited, New Delhi, 2011

(Advanced Reading)

- 1. C. Chambers and A. K. Holliday, *Modern Inorganic Chemistry*, First edition, Butterworth and Co., Sussex, 1975.
- 2. Gary L Miessler and Donald A Tarr, *Inorganic Chemistry*, Third edition, Pearson Prentice Hall.
- 3. G. R. Choppin, and J-O. Liljenzin, and J. Rydberg, *Radiochemistry and Nuclear chemistry*, Butterwoth-Heinemann, Woburn, 2002.
- 4. P. A. C. McPherson, *Principles of Nuclear Chemistry*, World scientific, Singapore, 2017.

SEM IV CH416-Organic Chemistry - III Hrs/week – 3 (Credits 3)

Objectives

- Understanding the fundamentals of organic spectroscopy.
- Understanding Aromatic compounds.
- Understanding the reactivities of carbonyl compounds.
- Learning radical reactions.

Unit 1 Radical reactions

1.1 Radical reactions of alkanes, poor reactivity of alkanes, chlorination and bromination of alkanes.

9 hours

- 1.2 Radical stability and alkyl substituents, distribution of products and reactivity selectivity principle, formation of explosive peroxides, addition of radicals to alkenes, stereochemistry of radical substitution and addition reactions
- 1.3 Radical substitution of Benzylic and allylic hydrogens.

Unit 2 Organic Spectroscopy 1

- 2.1 Mass spectrometry, mass spectrum and fragmentation, isotopes in mass spectrometry, high resolution mass spectrometry, fragmentation pattern of functional groups.
- 2.2 Infrared spectroscopy, infrared spectrum functional group and fingerprint region, characteristic absorption bands, intensity of absorption bands, position of absorption bands: effect of bond order, delocalization, electron donation, withdrawal and hydrogen bonding. OH and CH absorptions.
- 2.3 Shape of absorption bands and absence of absorption bands, interpreting and IR spectrum.

Unit 3 Aromaticity

- 3.1 Aromaticity, unusual stability of aromatic compounds, two criteria for aromaticity, applying the criteria for aromaticity, aromatic heterocyclic compounds, chemical consequences of aromaticity,
- 3.2 Anti-aromaticity, molecular orbital description of aromaticity.
- 3.3 Reactivity of Benzene, electrophilic aromatic substitution reactions: halogenation, sulfonation, nitration, Friedel crafts acylation, alkylation. Reduction of acylated benzene to alkyl benzene.

Unit 4 Substituted Benzenes

- 4.1 Reaction of Substituted Benzenes: Chemical conversion of substituents on the benzene ring, effect of substituents on reactivity.
- 4.2 Effect of substituents on orientation of incoming groups, on pKa. Ortho-Para ratio, substituent effects. Synthesis of mono and disubstituted, substituted benzenes using diazonium salts.
- 4.3 Arene diazonium as an electrophile, Reaction of Amines with Nitrous acid, Nucleophilic aromatic substitution an addition elimination reaction and Benzyne reaction. Dyes: Phenolpthlaein, Methyl orange and Fluorescein.

Unit 5 Carbonyl compounds 1

- 5.1 Carbonyl compounds, Nomenclature of carbonyls, Structure of carboxylic acid and their derivatives, Physical properties of carbonyl compounds.
- 5.2 Reactivity of carbonyls, relative reactivities of carboxylic acids and their derivatives. General mechanism of nucleophilic addition and elimination reaction.
- 5.3 Reaction of acyl halides, anhydrides, esters. Acid and base catalyzed hydrolysis of an ester and transesterification. Hydroxide ion hydrolysis of esters, evidence for nucleophilic addition elimination reaction of carbonyls.

Reference Books:

Text Book

1. Paula Yurkanis Bruice, Organic chemistry, 6th Edition, Prentice Hall, Illinois, 2011.

Further reading

- 2. R.T. Morrison and R. N. Boyd, *Organic chemistry*, 6th Edition, Prentice-Hall of India, New Delhi, 2008.
- 3. Leroy. G. Wade, *Organic chemistry*, 6th Edition, Pearson, New York, 2005.
- 4. Clayden, J Greeves, N and Warren, S, *Organic Chemistry*, 2nd Edition, Oxford University Press, New York, 2001.

9 hours

9 hours

9 hours

5. Loudon, Marc G, *Organic Chemistry*, 6th Edition, Oxford University Press, New York, 2016.

Outcomes

- Correlate reactants and products using spectroscopy.
- Knowledge on Aromacity and reactivity.
- Knowledge of the nature of carbonyl compounds.

SEM IV CH417-Physical Chemistry - II Objectives

- To understand the important laws of thermodynamics and their implications in chemical systems
- To learn the importance of chemical potential and its significance
- To understand the basic concepts and importance of phase equilibria
- To learn the basics of colloids, surfactants and solutions

Unit – I Thermodynamics - II

- 1.1 Need for second Law-Spontaneous Process- Cyclic Process- Carnot cycle- Concept of entropy-Entropy changes in reversible and irreversible process-
- 1.2 Statement of second law -entropy of mixture of ideal gases, entropy of mixing-physical significance of entropy
- 1.3 Helmholtz and Gibbs free energy- Maxwell relations-Criteria for spontaneity and equilibrium-Gibbs- Helmholtz equation-Chemical potential
- 1.4 Gibbs- Duhem equation- Variation of chemical potential with temperature and pressure -Chemical potential in a system of ideal gas-Third Law- Importance of third law, Testing and validity of third law. Residual entropy

Unit II Chemical Equilibrium:

- 2.1 State of chemical equilibrium Characteristics and experimental verification of chemical equilibrium. Law of Mass action Law of chemical equilibrium
- 2.2 Types of equilibrium constants, Relationship between Kp, Kc and Kx Applications of equilibrium constant with solved problems.
- 2.3 Free energy change criterion of spontaneity (Problems). Thermodynamic treatment of chemical equilibrium, De Donder's Concept- Chemical affinity. Thermodynamic relations for chemical affinity.
- 2.4 Van't Hoff reaction isotherm (problems)-Van't Hoff equation (Temperature dependence) (problems) Le Chatelier's principle Effect of temperature, pressure and concentration and applications

Unit - III Phase Rule

- 3.1 Explanations of terms Phase, components and Degrees of freedom. Equilibrium Criteria for equilibrium Thermal, mechanical and chemical equilibrium. Thermodynamic derivation of Phase rule.
- 3.2 Clausius-Clapeyron Equation and its application in phase transition-Phase diagram One component system Water and sulphur with polymorphism.
- 3.3 Two component system– Reduced phase rule, types of two component system involving solid liquid equilibria General features of two component system Colling curve method.
- 3.4 Simple eutectic system: Pb– Ag system. KI water system freezing mixture

Unit – IV Phase Equilibria II and Colloids:

12 Hours

NAAC 5th CYCLE

12 Hours

12 Hours

12 Hours

Hrs/week – 4 (Credits 4)

- 4.1 Two components with compound formation Congruent Melting point Ferric chloride
 water system (Activity Construction of Mg Zn system phase diagram) Incongruent Melting point Na K system
- 4.2 Colloids Types of colloids Origin of charge on colloids- electrical double layer-Electrokinetic properties (Electrophoresis, electro osmosis)
- 4.3 Surfactants: Classification- Micelle and reverse micelle formation- shape and structure of micelles- critical micelle concentration, aggregation number
- 4.4 Factors affecting CMC in aqueous media- Thermodynamics of Micellization (no derivation)

Unit – V Solutions

12 Hours

- 5.1 Thermodynamics of ideal solutions: Ideal solutions, Henry', s law and Raoult's law, deviations from Raoult's law non-ideal solutions.
- 5.2 Temperature composition diagrams ideal liquid mixture (Toluene Benzene)-Nonideal mixture (water – ethanol and water – hydrogen chloride) – Distillation of immiscible liquids.
- 5.3 Partially miscible liquids: Phenol Water, Triethylamine Water and Nicotine Water systems.
- 5.4 Nernst distribution law Thermodynamic derivation-limitations, Applications of Nernst distribution law- Solvent extraction and Determination of Hydrolysis constant.

Text Books:

- 1. B. R. Puri, L. R. Sharma and M. S. Pathania, *Principles of Physical Chemistry*, 47th Edition, Vishal Publishing Co, Jalandar, 2016.
- 2. R.L. Madan, *Physical Chemistry*, Mc Graw Hill Education Pvt. Ltd. 2015.

Reference:

1. Arun Bahl, B.S. Bahl. G.D.Tuli, Essentials of Physical Chemistry, S. Chand Publications

2. A.S. Negi and S.C. Anand, *A text book of Physical Chemistry*, Wiley Eastern Ltd, New Delhi, 1984.

Learning Outcome:

- Relate and interpret the various laws of thermodynamics
- Know the relevance of free energy in chemical reactions
- Discuss the fundamental aspects of chemical equilibrium
- Illustrate the behaviour of chemical mixtures using suitable phase diagrams
- Correlate the type of colloids with its properties
- Identify and distinguish the types of solutions

Semester III & IV PCH408-Qualitative Inorganic Analysis 3 Hrs/week (3 Credits/ sem) Objectives:

- To enable the student to systematically identify the cations and anions present in a inorganic mixture
- To know the appropriate chemical procedures and apply them to prepare some familiar complexes

1. Qualitative Inorganic Mixture Analysis:

- 1.1 Analysis of mixture containing two cations and two anions of which one will be interfering.
- 1.2 Anions: Chloride, Carbonate, Sulphate, Nitrate, Borate, Fluoride, Oxalate, and Phosphate.
- 1.3 Cations: Lead, Copper, Bismuth, Cadmium, Iron, Aluminium, Zinc, Manganese, Cobalt, Nickel, Calcium, Strontium, Barium, Ammonium and Magnesium.

2. Inorganic Preparations

- 2.1 Tetrammine Copper(II) Sulphate
- 2.2 Hexammine Nickel (II) Chloride
- 2.3 Tris (thiourea) Copper(II) Chloride
- 2.4 Potassium trioxalato ferrate (III)

References

- 1. V. Venkateswaran, R. Veerasamy, A.R. Kulandaisamy, *Basic principles of Practical Chemistry*, S.Chand publications, New Delhi, 2002.
- 2. V. V. Ramanujam, *Inorganic Semimicro Qualitative Analysis*, 3rd Edition, The National Publishing Company, 2003.
- 3. A.O, Thomas. *Practical Chemistry*, 6th Revised Edition, Sharada Press, 1995.

Semester – III ACH308-Allied Chemistry-I (Maths and Physics)

Learning Objectives

- 1. To learn the electronic configuration of atoms, periodicity of elements and Chemical bodings
- 2. To understand the Structure and bonding of Co-ordination compounds
- 3. To learn the principles of Organic Chemistry, Organic reactions and mechanism

Unit I Atomic Structure

12 Hours

4 Hrs/week (2Credits)

- 1.1 Electronic configurations of the elements, Aufbau principle, quantum numbers and Pauli's exclusion principle.
- 1.2 Hund's multiplicity rule for filling electrons in various orbitals, Stability of half-filled and completely filled orbitals, effective nuclear charge.
- 1.3 Shapes of s, p, d orbitals s, p, d and f block elements classification and characteristic properties.
- 1.4 Periodicity of properties Definition and periodicity of the following properties Atomic radii factors affecting atomic radii ionic radii factors affecting ionic radii. Ionisation potential factors affecting ionisation potential Electron affinity factors affecting electron affinity Electronegativity factors affecting electronegativity Pauling scale

Unit II Chemical Bonding

- 2.1 Ionic Bonding: General characteristics of ionic bonding. Energy considerations in ionic bonding, lattice energy and solvation energy and their importance in the context of stability and solubility of ionic compounds
- 2.2 Born-Haber cycle and its applications, Polarizing power and polarizability Fajan's rules, ionic character in covalent compounds
- 2.3 Covalent bonding: Lewis theory, Octet theory, VSEPR theory and its applications geometries of BCl₃, H₂O, ClF₃, IF₇ and XeF₆ molecules.
- 2.4 VBT-Hybridization CH₄, C₂H₄, C₂H₂- BeCl₂, BF₃, NH₃, H₂O, SF₆

Unit III Co-ordination Chemistry

- 3.1 Double salts and coordination compounds-Definition of terms Types of ligands -IUPAC Nomenclature of coordination compounds.
- 3.2 Werner's theory –Sidgwick's concept and EAN rule
- 3.3 Valance Bond theory and its applications to $[Co(NH_3)_6]^{3+}$, $[Fe(CN)_6]^{3-}$, $[CoF_6]^{3-}$, $[Cr(H_2O)_6]^{2+}$, $Ni(CO)_4$, $[MnCl_4]^{2-}$, $[Ni(CN)_4]^{2-}$, $[Cu(NH_3)_4]^{2+}$, limitations of VBT
- 3.4 Chelation and stability of coordination compounds. Structure and functions of Haemoglobin and Chlorophyll

Unit IV Principles of Organic Chemistry

- 4.1 Electronic Displacement Effects: Inductive Effect, Electromeric Effect, mesomeric effect and Hyperconjugation
- 4.2 Strength of organic acids and bases Inductive Effect & mesomeric effect.
- 4.3 Cleavage of Bonds: Homolysis and Heterolysis, formation of reactive intermediates Carbocations, Carbanions and free radicals
- 4.4 Structure, shape and reactivity of reactive intermediates: Carbocations, Carbanions and freeradicals

Unit V Organic reaction and mechanism

5.1 Preparation and properties of alkyl halides

- 5.2 Types of Nucleophilic Substitution reactions in alkyl Halides (SN1, SN2)–Factors influencing SN1/SN2
- 5.3 Alcohols- Preparation of alcohols using Grignard reagent, Ester hydrolysis, Reduction of aldehydes, ketones, carboxylic acid and esters. Reactions of alcohols with sodium, HX (Lucas test), esterification, oxidation (with PCC, alk. KMnO₄, acidic dichromate, conc. HNO₃)
- 5.4 Aromaticity- Criteria for aromaticity- preparation and properties of benzene-Electrophilic substitution in benzene Mechanism of aromatic nitration, sulphonation, halogenations and Friedel Crafts alkylation and acylation

Learning Outcomes

Students will be able to write the electronic configuration of atoms, able to classify the elements as main group elements, transition elements, and f block elements, able to recognize the type of Chemical bond formed and correlate the properties of molecules with the bond type, able to know the basic principles of organic chemistry, the organic reactions and mechanism.

References:

- 1. Concise Inorganic Chemistry by J.D. Lee, Wiley publications
- 2. Principles of Inorganic Chemistry by Puri, Sharma, Vishal Publications
- 3. Modern Inorganic Chemistry, R.D. Madan, S. Chand publications
- 4. Concise Coordintion Chemistry by R. Gopalan, Vikas publications
- 5. Organic Chemistry by Robert Thornton Morrison, Robert Neilson Boyd, Pearson

12 Hours

12 Hours

publications

- 6. Organic Chemistry by Jain, Sharma, Vishal Publications
- 7. Reactions, Rearrangements and Reagents by S N Sanyal, Bharati Bhawan Publications

Semester - IV ACH409-Allied Chemistry - II (Maths and Physics)

4 Hrs/week (2Credits)

Learning Objectives

- 1. To understand the principles of rate of chemical reactions and thermodynamics
- 2. To understand the basic electrochemistry, pH and buffer solutions
- 3. To learn the basic nuclear chemistry and its applications
- 4. To learn the chemistry of carbohydrate, amino acids, proteins and enzymes

Unit I Chemical Kinetics

- 1.1 Introduction to reaction rates Rate of a Reaction-Rate law-Reactant and Product Concentrations as a Function of Time - Average, Instantaneous rates -Factors affecting rate of a Chemical reaction
- 1.2 Molecularity of a reaction- order of a reaction- Determining the Order of a Reaction by graphical method, Rate equation method and Ostwald isolation method.
- 1.3 Derivations of rate constant for Zero, First, and Second (2A→ products) order reactions – Half-life Period- Study of kinetics by Volumetric method (Ester hydrolysis) and Polarimetric method (Inversion of Sucrose)
- 1.4 Effect of temperature on reaction rate temperature coefficient concept of activation energy- Arrhenius equation.

Unit II Thermodynamics

- 2.1 Scope and limitations of thermodynamics-Terminologies in thermodynamics, types of system, surroundings, types of processes
- 2.2 First law of thermodynamics and internal energy, enthalpy and enthalpy of processes, limitations of first law. Zeroth law of thermodynamics
- 2.3 Second law of thermodynamics, Carnot engine and calculation of efficiency
- 2.4 Concept of entropy, entropy as criteria for spontaneity, statement of Third law of thermodynamics.

Unit III Electro Chemistry and Ionic Equilibria

- 3.1 Electrolytic conduction: Conductors, types of conductors. Specific conductance, equivalent conductance and molar conductance, variation of conductance with concentration, molar or equivalent conductance at infinite dilution, Kohlraush's law
- 3.2 Applications of conductance measurements: Determination of Dissociation constant of weak acids, Solubility of sparingly soluble salt, Conductometric titrations: Strong acid Vs strong base, weak acid Vs strong base, Strong acid Vs weak base, mixture of strong acid and weak acid Vs strong base, Precipitation titration.
- 3.3 pH and pOH: Definition and explanation. Calculation of pH/pOH of weak acids and bases
- 3.4 Buffer solutions: definition and examples- Explanation of buffer action of acid buffer and basic buffer Henderson Hasselbalch equation

Unit IV Nuclear Chemistry

- 4.1 Stability of nucleus-N/P ratio, Binding energy-Natural and Artificial Radioactivity-Types of radioactive rays, difference between chemical and nuclear reactions
- 4.2 Rate of disintegration, half life period, and average life period-Representation of nuclear reactions-calculation of nuclear Q value-group displacement law

12 Hours

CRITERION I

NAAC 5th CYCLE

12 Hours

12 Hours

- 4.3 Nuclear Fission, atom bomb and Nuclear reactor -Nuclear Fusion, hydrogen bomb and stellar energy
- 4.4 Carbon and rock dating -Applications of radioisotopes in agriculture, medicine, and industry

Unit V Bio molecules

12 Hours

- 5.1 Carbohydrates: Classification, Cyclic Structures of Monosaccharides (The Cyclic Hemiacetal Form of Glucose/Fructose)
- 5.2 Epimerization and the Enediol Rearrangement-Reduction of monosaccharides -Oxidation of Monosaccharides-Reactions with Phenylhydrazine- Inter-conversion of glucose to fructose and fructose to glucose
- 5.3 Amino acids: Classification, standard amino acids, physical and chemical properties of glycine, Proteins-classification based on function, primary and secondary structure of protein
- 5.4 Enzymes- classification-Active sites-Lock and Key model-Induced fit model-Conformational selection model- Michaelis Menten equation-Linewaeaver-BurK Plot

Learning outcomes

Students will be able to understand the basic principles of Chemical kinetics, Thermodynamics, Electrochemistry, and Ionic equilibria. They will understand the stability of atoms and the rate of disintegration and applications of nuclear chemistry. They will be able to know the functions and structures of biomolecules

References:

- 1. Principles of Physical Chemistry by Puri, Sharma, Pathania, Vishal Publications
- 2. Physical Chemistry by Arun Bahl, S. Chand Publications
- 3. A Textbook of Physical Chemistry by A. S. Negi and S. C. Anand, New age international publications.
- 4. Organic Chemistry by Jain, Sharma , Vishal Publications
- 5. Organic Chemistry by Wade ,Pearson publications
- 6. Lehninger Principles of Biochemistry Nelson, Cox, WH Freeman publications
- 7. Organic Chemistry by Paula Yurkanis Bruice, Pearson publications
- 8. Modern Inorganic Chemistry by R.D. Madan, S.Chand publications
- 9. Principles of Inorganic Chemistry by Puri, Sharma, Vishal Publications

Semester - III & IV PACH209/PACH409Allied Chemistry Lab Work (Mathematics, Physics and Biochemistry,)2 Hrs / week (4 Credits)

Objectives

- To learn the basics of analysis involved in estimating the amount of substances.
- To acquire the practical knowledge about the analysis of organic compounds

Volumetric Analysis

Estimation of Hydrochloric acid using std. Oxalic acid. Estimation of NaOH using std. Na₂CO₃ Estimation of FeSO₄ using std. FAS solution Estimation of Oxalic acid using std. FAS. Estimation of Fe²⁺ using diphenylamine as indicator.

Qualitative Organic Analysis

Systematicanalysis of organic compounds containing one functional group and characterization by confirmatory tests - Aromatic aldehydes, ketones, carbohydrate, Aromatic carboxylic acid, phenol, aromatic primary amineand amides

References

- 1. V. Venkateswaran, R. Veerasamy, A.R. Kulandaisamy, Basic principles of Practical Chemistry, S.Chand publications, New Delhi, 2002.
- 2. A.O, Thomas. Practical Chemistry, 6th Revised Edition, Sharada Press, 1995
- 3. J. N. Gurtu And R. Kapoor, Advanced Experimental Chemistry, Vol. I Physical Chemistry, Vol. II Inorganic Chemistry, Vol. III Organic Chemistry, Organic Reactions & Reagents [B.Sc., (Hons.) & M.Sc.], Himalayan Publishers, 1974.

SEM V CH545- Organic Chemistry - IV

Course Objectives

Understanding the reactivities of carbonyl compounds. Understanding oxidation and reduction reactions.

Unit 1 Carbonyl compounds 2

- 1.1 Soaps, detergents and micelles. Reactions of carboxylic acids, amides.
- 1.2 Hydrolysis of amides catalyzed by esters, hydrolysis of imides synthesis of primary amines, hydrolysis of nitriles.
- 1.3 Activation of carboxylic acids. Dicarboxylic acids and their derivatives.
- 1.4 Relative reactivities of carbonyls, reactivities of aldehydes and ketones.

Unit 2 Carbonyl compounds 3

- 2.1 Reaction of carbonyls with Grignard reagents, acetylides, hydride.
- 2.2 Reaction of aldehydes and ketones with hydrogen cyanide, amines and amine derivatives, formation of imine derivatives.
- 2.3 Wolf-Kishner reduction, Enamine formation, reductive amination, Reaction of aldehydes and ketones with water and alcohols.
- 2.4 Protecting groups. Addition of sulphur nucleophiles, Wittig reaction.

Unit 3 Carbonyl compounds 4

- 3.1 Stereochemistry of nucleophilic additions Re and Si faces. Nucleophilic addition to α , β unsaturated aldehydes, ketones and carboxylic acid derivatives.
- 3.2 Acidity of α hydrogen in carbonyl compounds, keto-enol tautomers, keto enol interconversion, reactivities of enolates and enols.
- 3.3 Halogenation at α carbon of aldehydes, ketones and carboxylic acids.
- 3.4 LDA and formation of enolate ion.

Unit 4 Carbonyl compounds 5

- 4.1 Alkylation of α carbon of carbonyl compounds, Alkylation and acylation of α carbon using enamine intermediate. Alkylation of β - carbon Michael reaction.
- 4.2 Aldol addition forming β hydroxy aldehydes and β hydroxy ketones, dehydration of aldols forming α , β unsaturated aldehydes, and ketones, crossed aldol addition.
- 4.3 β keto ester formation by Claisen condensation, crossed Claisen condensation, intramolecular condensation and addition reactions, Robinson annulation, decarboxylation of carboxylic acids with carbonyl at 3-position.

12 hours

12 hours

Hrs/week – 4 (Credits 4)

12 hours

4.4 Carboxylic acids from Malonic ester, methylketone from acetoacetic ester.

Unit 5 Oxidation and Reduction

- 5.1 Oxidation and reduction reactions an overview, reduction reactions, chemoselective reactions.
- 5.2 Oxidation of alcohols, oxidation of aldehydes and ketones, oxidation of alkenes to 1,2 diols, oxidative cleavage of 1,2 diols, oxidative cleavage of alkenes, functional group interconversion.
- 5.3 Acid base properties of amines, amines as bases and nucleophiles. Aromatic five membered heterocycles.
- 5.4 Aromatic six membered heterocycles, Natural roles of heterocycles.

Reference Books:

Text Book

1. Paula Yurkanis Bruice, Organic chemistry, 6th Edition, Prentice Hall, Illinois, 2011.

Further reading

- 2. R.T. Morrison and R. N. Boyd, *Organic chemistry*, 6th Edition, Prentice-Hall of India, New Delhi, 2008.
- 3. Leroy. G. Wade, Organic chemistry, 6th Edition, Pearson, New York, 2005.
- 4. Clayden, J Greeves, N and Warren, S, *Organic Chemistry*, 2nd Edition, Oxford University Press, New York, 2001.
- 5. Loudon, Marc G, Organic Chemistry, 6th Edition, Oxford University Press, New York, 2016.

Outcomes

Knowledge on carbonyl compounds and their reactivities. Knowledge about redox reagents in organic reactions.

SEM V CH546-Inorganic Chemistry - III Hrs/week – 4 (Credits 4)

Course Objectives:

To study the chemistry of main groups elements

To understand the variation in the periodic behavior

To learn the methods of extraction of lanthanides and actinides

Unit-1 Chemistry of Group 16

- 1.1 Group 16- chalcogens: general properties, electronic configuration, oxidation states. Oxides- classification, structure and properties.
- 1.2 Oxo-acids and peroxo-acids of Sulphur.
- 1.3 Hydrogen peroxide and Hydrogen sulphide- preparation and properties.
- 1.4 Allotropes of Oxygen and Sulphur. Chemistry of Ozone.

Unit-2 Chemistry of Halogens and Noble gases

- 2.1 Group 17: electronic configuration, oxidation states, ionization energies, and electron affinity. Hydrogen halides- preparation, properties and uses. Halides- ionic, molecular and bridging.
- 2.2 Preparation and properties of Oxo-acids- Hypohalous acids, halous acids, Halic acids and perhalic acids. Pseudo halogens and halides.
- 2.3 Preparation, properties and structure of Interhalogen compounds types; ICl, BrF_3 , ClF_5 and IF_7 .
- 2.4 Noble gases: Xenon clatharates. Preparation properties and structure of Xenon fluorides.

12 hours

12 hours

- 3.1 General group trends, electronic configuration.
- 3.2 General characteristics: metallic character, molar volume and densities, ionisation energies, variable valency, stability of oxidation states, and colour.
- 3.3 Magnetic properties- para-magnetism, diamagnetism and effective magnetic moment, catalytic properties, determination of magnetic properties
- 3.4 Comparison between first, second and third transition series. (Ionic radius, coordination number, metal – metal bonding and oxidation state)

Unit-4 Chemistry of lanthanides and actinides

- 4.1 Electronic structure, configuration and position of lanthanides and in the periodic table.
- 4.2 Properties of lanthanides and actinides: basic character, solubility, double salts and chemical reactivity
- 4.3 Chemical properties of lanthanides and actinides-oxidation state, magnetic properties, colour and spectral properties.
- 4.4 Lanthanide and actinide contraction and its consequences.

Unit-5 Extraction of Lanthanides and Actinides

12 hours

- 5.1 Extraction of lanthanides from monazite sand
- 5.2 Separation of the lanthanides (Precipitation, fractional crystallization, complex formation, solvent extraction, valency change). Uses of lanthanides.
- 5.3 Extraction of Thorium and uranium and compounds of thorium and uranium
- 5.4 Comparative studies of lanthanoids and actinoids with transition elements.

Learning Outcomes

Identify the chemistry of p-block elements (Group 16 and 17) and noble gases

- Explain the periodic trends, chemical reactivity and physical properties of d and f-block elements
- List out important inorganic compounds of d and f block elements, their extraction and applications

References

(Text Book)

- 1. R. D. Madan, Modern Inorganic Chemistry, Second edition, S. Chand publications, New Delhi, 2000.
- B. R. Puri, L. R. Sharma and K. C. Kalia, Principles of Inorganic Chemistry, 33rd 2. Edition, Vishal Publishing Co, Jalandar, 2004.
- 3. 1. J. D. Lee, *Concise Inorganic Chemistry*, Chapman and Hall: London, 1961.

(Advanced Reading)

- 1. C. Chambers and A. K. Holliday, Modern Inorganic Chemistry, First edition, Butterworth and Co., Sussex, 1975.
- 2. Gary L Miessler and Donald A Tarr, Inorganic Chemistry, Third edition, Pearson Prentice Hall.
- 3. A. G. Sharpe and C. E. Housecraft, *Inorganic Chemistry* Vol-I, 3rd edition, Pearson prentice Hall, New York, 2008.

CH547-Physical Chemistry - III Hrs/week – 4 (Credits 4) SEM V

Objectives

CRITERION I

To have a good foundation about the quantum chemistry and learn the application to simple system

To learn the concepts regarding chemical kinetics and apply them for kinetics related problems in chemical reactions

To learn the importance of photophysical and photochemical processes

Unit – I Fundamentals of quantum Chemistry

- 1.1 Need for quantum mechanics-Black body radiation, Quantum theory of radiation, Photoelectric effect.
- 1.2 Rutherford's model of atom and its failure, Bohr's theory of hydrogen atom, spectrum of hydrogen atom Sommerfeld theory
- 1.3 Dual behaviour of matter and radiation -de Broglie's relation, Davisson-Germar experiment, Compton effect, Heisenberg Uncertainty principle.
- 1.4 Solving One-dimensional wave equation for a standing wave-Separation of variables-Interpretation of results

Unit - II Quantum Mechanics

- 2.1 Schrodinger's wave equation-Eigen value/Eigen function-Postulates of Quantum mechanics –
- 2.2 Operators Algebra of operators commutative property Linear operator and Hermitian property momentum operator, KE operator, Hamiltonian operator.
- 2.3 Solution of Schrodinger's wave equation for simple systems: Free particle- Particle in one dimensional box (Origin of quantization)
- 2.4 Particle in one dimensional box (Expectation Values for momentum and position, Verification of Heisenberg's Uncertainty Principle)-Applications of particle in a box and particle in three dimensional box.

Unit - III Chemical Kinetics I

- 3.1 Introduction to reaction rates Rate of a Chemical Reaction-Reactant and Product Concentrations as a Function of Time - Average, Instantaneous, and Initial Reaction Rates -Factors affecting rate of a reaction (nature of reactants, concentration of reactants, effect of temperature, effect of catalyst)-Molecularity-Elementary steps-Order of a reaction-Rate Determining Step-Determining the Order of a Reaction by changing concentration of reactants (including numerical problems)
- 3.2 Derivations of Zero, First, Second (2A® products & A +B® products)
- 3.3 Third order reactions (3A[®] products)–Half-life (Zero/First/Second/Third)- study of kinetics by Volumetric (Ester hydrolysis) and Polarimetric (Inversion of Sucrose)
- 3.4 Determination of order of the reactions-Graphical method, rate equation method, halflife method and Ostwald's method.
 *Numerical Problems related to above topics

*Numerical Problems related to above topics

Unit - IV Chemical Kinetics II and Catalysis

- 4.1 Effect of temperature on reaction rate temperature coefficient concept of activation energy- Arrhenius equation.
- 4.2 Theories of reaction rates: Bimolecular collision theory Transition state theory Lindemann's unimolecular theory.

12 Hours

12 Hours

12 Hours

- 4.3 Catalysis General characteristics. Activation energy (for catalyst/ without catalyst). Theories of catalysis Adsorption theory / Intermediate compound formation theory.
- 4.4 Enzyme catalysis: theory Mechanism and kinetics of enzyme catalysed reaction-Michaleis-Menton equation – Lineweaver-Burk Plot
 *Numerical Problems related to the above topic

Unit - V Photochemistry and Adsorption

12 Hours

- 5.1 Interaction of radiation with matter- Difference between thermal & photochemical processes Laws of photochemistry: Grotthus Draper law, Stark Einstein law-Jablonski diagram depicting various processes occurring in the excited state.
- 5.2 Qualitative description of fluorescence, phosphorescence, non-radioactive processes (internal conversion, inter system crossing), quantum yield, photosensitized reactions.
- 5.3 Adsorption Distinction between physical and chemical adsorption-Factors influencing adsorption-
- 5.4 Adsorption isotherm Freundlich isotherm. Langmuir isotherm- theory and derivation.

Text Books:

- 1. B. R. Puri, L. R. Sharma and M. S. Pathania, *Principles of Physical Chemistry*, 47th Edition, Vishal Publishing Co, Jalandar, 2016.
- 2. R.L. Madan, *Physical Chemistry*, Mc Graw Hill Education Pvt. Ltd. 2015.

Reference:

- 1. Arun Bahl, B.S. Bahl. G.D.Tuli, Essentials of Physical Chemistry, S. Chand Publications
- 2. A.S. Negi and S.C. Anand, A text book of Physical Chemistry, Wiley Eastern Ltd, New Delhi, 1984.

Learning Outcome:

Explain the fundamental principles of quantum mechanics

Describe the kinetics of chemical reactions

Explain the characteristics of catalysis

Describe the various photophysical and photochemical processes.

Identify the different types of adsorption

SEM V CH548-Analytical Chemistry - II

Hrs/week – 4 (Credits 4)

Objectives:

To study the basics, principles and instrumentation of spectroscopy.

To learn the basics, principles of polarography and amperometric techniques.

Unit - I: Colorimetric Analysis, UV-Visible Spectroscopy and Mass Spectrometry **12 Hours**

- 1.1 Introduction to spectroscopy-spectrum-Electromagnetic Radiation-Planck's equationwavelength-frequency-wave number.
- 1.2 Mass Spectrometry-Principle-Instrumentation- Dampster spectrometer. McLaffertary rearrangement - The Mass spectrum-fragmentation with illustration: CH₄, C₂H₅OH, CH₃COCH₃, Determination of molecular formula and molecular weight: Example-Acetic acid.
- 1.3 Colorimetric analysis-laws of colorimetry-photoelectric Colorimeter-Estimation of Fe and Ni. Determination of composition of complex Job's Methods-Example: Ni-EDTA complex.
- 1.4 UV-Visible Spectroscopy-Types of transition in Organic Compounds-Types of absorption band-chromophore-auxochrome-bathochromic shift, hypsochromic shift, hyperchromic shift and hypochromic shift. Instrumentation-single and double beam and applications of simple systems.

Unit - II: IR and Raman Spectroscopy

12 Hours

- 2.1 IR Spectroscopy-theory-types of Vibrations-Example: H₂O and CO₂.
- 2.2 Instrumentation and sampling techniques.
- 2.3 Applications: Structure of NO₂, study of Hydrogen Bonding-Identification of simple organic compounds: alcohols, acids, amines, esters, ketones and unsaturated compounds.
- 2.4 Raman Spectroscopy-theory-advantages over IR Spectroscopy. Instrumentation and sample Handling-Depolarization Effect-Mutual Exclusion principle, applicationsstructure of CO₂, nitrous oxide and mercurous chloride.

Unit - III: NMR and ESR Spectroscopy

- 3.1 NMR Principle: theory-allowed orientation-spin states and relaxation- chemical shift.
- 3.2 Factors affecting chemical shift, spin-spin coupling, and hydrogen exchange.
- 3.3 Instrumentation and sample Handling-Applications: Structural identification-Examples: 1-Bromo Propane, 2-Bromo Propane, Toluene, Phenol and Vinyl Chloride.
- 3.4 ESR Principle-Theory-Selection rule for Transition-Instrumentation- Zero Field Splitting-Hyperfine splitting. Applications-ESR of simple organic radicals: CH₃-ESR of V^{4+} . Mn²⁺ and Cu²⁺ ions.

Unit - IV: AAS and AES

- 4.1 Atomic absorption Spectroscopy-Principle-Advantages and disadvantages of AAS.
- 4.2 Instrumentation of AAS, Interferences in AAS. Applications of AAS-Determination of Mg in water and Lead in Petrol.
- 4.3 Atomic Emission Spectroscopy- Principle of Flame photometry, AES-Principle-Advantages and Disadvantages.
- 4.4 Instrumentation of AES, Applications- Comparison of AAS and AES.

Unit - V: Polarography and Amperometry

5.1 Polarography-principle and instrumentation -current-voltage curves

12 Hours

12 Hours

- 5.2 Evaluation of Polarographic waves-half-wave potential, Ilkovic equation.
- 5.3 Applications of polarography for organic and inorganic systems.
- 5.4 Amperometry- Principle-Instrumentation-Types of curves. Advantages of amperometric titrations-applications of amperometric titrations.

References

- 1. R.Gopalan, P. S. Subramanian and K. Rengarajan, *Elements of analytical chemistry*, 3rd Edition., Sultan Chand, New Delhi, 2003
- 2. A. K. Srivatsava and P. C. Jain, *Chemical Analysis and Instrumental Approach*, 3rdEdition, S.Chand and Company Ltd., New Delhi, 2010.
- 3. A. I. Vogel, A text book of quantitative inorganic analysis, Longman, New York, 1985.
- 4. H. H. Willard, L. L. Merritt and J. A. Dean, *Instrumental methods of analysis*, 7thEdition., East West Press, New Delhi, 1986.
- 5. D. A. Skoog and D. M. West, *Principles of instrumental analysis*, Holt Saunders, Tokyo, 2001.
- 6. Gurdeep R Chatwal, *Instrumental Methods of Chemical Analysis*, 5thEdition. Himalaya Publications, 2005.
- 7. S. M. Khopkar, *Basic Concepts of Analytical Chemistry*, New Age Publishers, 2ndEdition. 2000.
- 8. V. Suryanarayanarao, *Polarography and Allied techniques*, University Press, 2002.

Learning Outcomes

To learn and understand the basic analytical techniques and their applications

To understand the basic principles that makes each analytical technique possible and useful

Semester - V CH549A-Elective-I Pharmaceutical Chemistry 3 Hrs/Week (2 Credits)

Objectives

To acquire a sound knowledge about the chemistry of drugs and their mechanism of action.

To learn about various types of diseases, their cause and cure through conventional and modern medicine.

Unit - I: Pharmacology

- 1.1 Introduction: Important terminologies used in medicinal chemistry Drugs, Dose, Pharmacology, Pharmacopoeia, therapeutics, toxicology, chemotheraphy, pharmacophore, metabolite, antimetabolite and mutation. Naming of drugs: Chemical name, proprietary name and non proprietary name with suitable examples.
- 1.2 Modes of administration of drugs: Enteral routes: oral, buccal, rectal. Parenteral routes: intradermal, subcutaneous, intramuscular, intravenous, intraarterial, intrathecal, intraperitoneal, intramedullary, intraarticular, inhalation, topical (meanings Only) Enteral dose forms. Disadvantages of enteral and parenteral routes -Definition of LD50, ED50 and therapeutic index.
- 1.3 Drug Stability –causes of drug degradation and their prevention.
 - Hydrolysis (procaine, Chloramphenical, aspirin)
 - Oxidation (ascorbic acid, adrenaline)
 - Polymerisation (formaldehyde)
 - Decarboxylation (procaine)
 - Drug design: New drugs, Lead compounds, SAR method,

Unit - II: Viral Infections

9 Hours

- 2.1 General Pharmacology: Meaning of receptor, agonist, antagonist, partial agonist, pharmaco dynamics and pharmacokinetics. Process of drug adsorption, distribution, metabolism and excretion Plasma half life period and its significance.
- 2.2 Viral diseases and antiviral drugs: Small pox, jaundice, rabies, influenza and AIDS causes, symptoms and treatment. SARS / COVID / Antiviral Drugs obstacles in antiviral therapy Structure and uses of acyclovir, iodoxuridine, amantadine and zidovudine (AZT).
- 2.3 Protozoal Infections: malaria the four malarial parasites life cycle of malarial parasites antimalarials: chloroquine, primaquine and quinine.

Unit - III: Bacterial Infections

9 Hours

- 3.1 Bacterial Infections: Meaning of bacteristat and bacteriocide, Gram-positive and Gramnegative bacteria. Antibacterial agents: Structure, uses and side effects of pencillins, streptomycin, chloramphenicol and tetracyclines.
- 3.2 Sulphonamides: Preparation and uses of sulphanilamide, sulphapyridine, sulphadiazine, Sulphathiazole, sulphaguanidine and prontosil-mode of action of sulphadrugs –General side effects of sulphadrugs.
- 3.3 Tuberculosis cause, symptoms and treatment of TB, tetanus and typhoid

Unit - IV: Types of Drugs

9 Hours

- 4.1 Inflammation and anti-inflammatory drugs: Examples for steroidal and non-steroidal anti-inflammatory drugs, Antihistamines Uses and side effects,
- 4.2 Analgesics: Narcotic analgesics- Exaction, physiological action, uses and side effects of morphine. Synthetic analgesics: preparation and uses of pethidine and methadone. Antipyretic analgesics: preparation, physiological action, uses and side effects of aspirin and paracetamol.
- 4.3 Sleep and hypnotics: Meaning of sleep, somnambulism, insomnia hypnotics, sedatives, tranquillisers. Preparation, uses and side effects of benzodiazepines and barbiturates. Psychotropicdrugs: Psycho stimulants Caffeine, Amphetamine structure, adverse effects and detection of LSD, Drug abuse Drug dependence, Evil effects of alcohol, tobacco, cannabis.

Unit - V: Other Diseases

9 Hours

- 5.1 Epilepsy, Parkinsonism: Meaning, causes, Symptoms and treatment (two drugs for each.
- 5.2 Cancer : Meaning of cancer causes and symptoms Treatment-Surgery, Radiation Therapy, Chemotherapy Anti neoplastic agents, Alkylating agents (Nitrogen&Sulphur Mustards), Antimetabolites (mercaptopurines, Fluorourcil),
- 5.3 Diabetes: Meaning, kind, cause and symptoms. Hyperglycaemia and hypolglycaemiacarbohydrate metabolism, Insulin and its action, Types of diabetes mellitus, Treatment of diabetes- Insulin therapy. Hypoglycaemic agents (Sulphonyl urea and biguanidines).

References

- 1. A. Jayashree Ghosh, *Textbook of Pharmaceutical chemistry*, Rajendra ravindra printers pvt. Ltd., New Delhi, 2010.
- 2. James Cross land, Lewis, *Pharmacology*, 5th Edition, Churchill Livingstone Publications, New York.1980
- 3. D. Sriram, P. Yogeeswari, *Medicinal Chemistry*, Second edition, Pearson publications, 2007
- 4. Alex Gringauz, Introduction to Medicinal chemistry, Wiley India Pvt Ltd., New Delhi, 2011.

- 5. Burger. Medicinal Chemistry and Drug Discovery, Vol-1, Ed. M. E. Wolff, John Wiley, 1994.
- 6. Goodman & Gilman. Pharmacological Basis of Therapeutics, McGraw-Hill, 2005.
- 7. S. S. Pandeya & J. R. Dimmock, Introduction to Drug Design, New Age International, 2000.
- 8. D. Lednicer, Strategies for Organic Drug Synthesis and Design, John Wiley, 1998.
- 9. Graham & Patrick. Introduction to Medicinal Chemistry, 3rd edition, OUP, 2005.
- 10. Rama Rao Nadendla, Principles of Organic Medicinal Chemistry, 2nd Edition, New Age Publications, 2008.
- 11. Ashutosh Kar, Medicinal Chemistry, 2nd Edition, New Age Publications, 2000.

Semester - V CH549B-Elective-I Forensic Chemistry

Objectives

- To understand the basic knowledge about forensic.
- To learn how chemistry supports in crime scene investigation and detection.
- To understand the determination of the crime using serology and identification of drugs usage.

Unit-1 Introduction to forensic chemistry, and crime scene assessing 9 hours

- 1.1 Introduction-Forensic science, origin of forensic science, earlier and advancement in forensic science.¹ Crime Scene: Securing isolating, Photography, Search for evidence, Collecting and packing evidence.²
- 1.2 Physical Evidences: Identification, Comparison. Assessing significance and value of physical evidence.²
- 1.3 Cautions and Limitations in Dealing with Physical Evidence. Forensic databases (Fingerprint and DNA databases).²

Unit-2 Detection Using fingerprints and DNA Finger printing

- 2.1. History and Usage of fingerprints. Early Classification of finger prints. Adoption of fingerprinting. Fundamental Principles of fingerprinting. Classification of finger prints.²
- 2.2. Methods of detecting fingerprinting: fingerprint powders, Iodine fuming, and ninhydrin.² Powder test, chemical test and light test.¹
- 2.3. DNA Fingerprinting-Chemistry behind biology-Application of DNA Testing.¹ Forensic DNA Typing-Procedure for DNA Typing-Slot-blot Test-Yield Gel Method-Methods of DNA Typing.¹

Unit-3 Examining Matter, Light, Paint, and glass

- 3.1 Nature of matter, Elements and compounds. States of matter. Physical properties and basic units and measurements, Density and Refractive indexes.²
- 3.2. Paint Chemistry, Binders, pigments. Architectural coatings. Paint evidence interpretation, Analytical methods (microscopic examination, and infrared spectroscopy).³ Inorganic and Organic pigment analysis. Any one case studies on analyzing crime using paint analysis.³
- 3.3. Hairs and fibers-Forensic examination of Hair-Identification and comparison of hair-Forensic examination of fibers-types of fibers-Chemical composition Identification.²

Unit-4 Forensic Serology

- 4.1. Nature of Blood: Antigens and antibodies.² Type of Bloods, polymorphic proteins and isoenzymes.¹ Identification of bloods (redox reaction and microcrystal assays).³
- 4.2. Forensic Characterization of blood stains (color, Luminol and bluestar, and microcrystalline test).²

9 hours

9 Hours

NAAC 5th CYCLE

9 hours

3 Hrs/Week (2 Credits)

4.3. Species identification: Immunochromatographic assays and Crossed-Over Immunoelectrophoresis.³

Unit-5 Drug testing

- 5.1. Alcohol and Human Body, Role of Forensic toxicology-Toxicology of alcohol.² Testing Blood Alcohol Concentration. Field tests-Drunkometer, Alcometer, Breathanalyzer, Fuel cell-based device.¹ Lab Analysis-Gas Chromatography.²
- 5.2. Techniques used in Toxicology. Drug dependence, (Psychological and Physical). Societal aspects of drug usage.² Types of Drugs (narcotics, Hallucinogens, and depressants). Forensic drug analysis. Quantitative and qualitative determination.⁷ Confirmatory tests (FTIR, Chromatography and GC).¹
- 5.3. Testing for poisons-Confirmatory tests (FTIR, GC and Mass).¹ Detecting Nondrug Poisons(Heavy Metals and CO), Significance of Toxicological findings.²

Learning Outcome

The student can explain the importance of chemistry in forensic science. The student can opt forensic science as their career.

References

(Text Book)

- 1. David E. Newton, Forensic Chemistry, Facts on File Science library, New York, 2007.
- 2. Richard Saferstein, *An Introduction to Forensic Science*, 12th Edition, Pearson Education, New York, **2018**.
- 3. Lawrence Kobilinsk, *Forensic Chemistry Handbook*, John Wiley and Sons, New Jersy, **2012**.

(Further reading)

- 4. Jay. A. Siegal, *Forensic Chemistry Fundamentals and Applications*, Wiley Blackwell, West Sussex, **2016**.
- 5. Forenscis Laboratory Manual, The McGraw-Hill Companies.
- 6. William G. Eckert, *Introduction to Forensic Sciences*, 2nd Edition, CRC Press, New York, **1992**.
- 7. Steven B. Karch, *Toxicology and Clinical Pharmacology of Herbal Products*, Humana Press, New Jersy, **2000**.

Semester - V CH549C-Elective-I Bioinorganic Chemistry 3 Hrs/Week (2 Credits)

Objectives:

To understand the scope of bioinorganic chemistry

To learn the chemistry of metelloporphyrin, metelloenzyemes.

To know the significance of metals in medicine.

Unit - I: Scope of Bioinorganic Chemistry

- 1.1 Introduction to Inorganic elements in biological systems and cells.
- 1.2 Biologically important compounds amino acids, proteins, nucleotides, carbohydrates and lipids, basic bioenergetics.
- 1.3 Classification of enzymes. Biochemistry: Distribution, biological roles, active transport of cations across membranes, the sodium pump.

Unit - II: Metalloporphyrins

2.1 Structure and optical spectra; heme proteins.

9 Hours

9 Hours

- 2.2 Magnetic susceptibility, epr and electronic spectra; hemoglobin and myoglobin: molecular structures.
- 2.3 Thermodynamics and kinetics of oxygenation, electronic and spatial structures, synthetic oxygen carriers

Unit - III: Metalloenzymes

- 3.1 Copper enzymes, superoxide dismutase, cytochrome oxidase and ceruloplasmin.
- 3.2 Coenzymes; Molybdenum enzyme: xanthine oxidase;
- 3.3 Zinc enzymes: carbonic anhydrase, carboxy peptidase and interchangeability of zinc and cobalt in enzymes.

Unit - IV: Metals in Medicine

- 4.1 Metal deficiency and disease; toxicity of mercury, cadmium, lead, beryllium, selenium and arsenic.
- 4.2 Biological defence mechanisms; chelation therapy; metals used for diagnosis.
- 4.3 Enzyme and chemotherapy, platinum complexes as anticancer drugs, Pt-DNA binding.

Unit -V: Nitrogen fixation and photosynthesis

- 5.1 Nitrogenase enzyme: reactivity, reduction involving nitride / diazene intermediate,
- 5.2 Dinitrogen complexes and their reactivity in vitro nitrogen fixation.
- 5.3 Photosynthesis: Structure of chlorophyll, in green plants (Z- scheme), ATP synthesis,

References

- 1. S. J. Lippard & J. M. Berg. *Principles of Bioorganic Chemistry*, Panima Publ. Corpn., 2005.
- 2. E.-I. Ochiai. Bioinorganic Chemistry An Introduction, Allyn and Bacon Inc., 1977.
- 3. M. N. Hughes. *The Inorganic Chemistry of Biological Processes*, Wiley, 1981.
- 4. R.P. Hanzlik. *Inorganic Aspects of Biological and Organic Chemistry*, Academic Press, 1976.
- 5. K. Hussain Reddy, *Bioinorganic chemistry*, New Age International Publishers, 2007.
- 6. H. Kraatz & N. Metzler-Nolte, *Concepts and Models in Bioinorganic Chemistry*, Wiley, 2006.
- 7. I. Bertini, H. B. Gray, S. J. Dippard & J. S. Valentine, *Bioinorganic Chemistry*, Viva Books Pvt. Ltd., 2004.
- 8. A.W. Addison, W.R. Cullen, D. Dolphin & B.R. James, *Biological Aspects of Inorganic Chemistry*, John Wiley, 1977.
- 9. R.J.P. Williams & J.R.R.F. Dasilva. *New Trends in Bioinorganic Chemistry*, Academic Press, 1978.
- 10. A. E. Martel. *Inorganic Chemistry in Biology and Medicine*, ACS Symp. Series, ACS, 1980.
- 11. S. J. Lippard. Progress in Inorganic Chemistry: Bioinorganic Chemistry, Vol. 38, John Wiley, 1990.
- 12. N. Kaim & B. Schwederski. *Bioinorganic Chemistry: Inorganic Elements in the Chenistry of Life*, John Wiley, 1994.

Semester - V CH550A-Elective-II Applied Chemistry 3 Hrs/week (2 Credits)

Objectives:

To inculcate the latest sophisticated analytical techniques

To characterize the solid-state materials which found applications in day-to-day life.

Unit - I: Analysis of Redox Potentials

9 Hours

NAAC 5th CYCLE

9 Hours

9 Hours

- 1.1. Basic Principles of Voltammetry-Nernst Equation-Applications of Voltammetry-Applications of cathodic and anodic peak potentials and current.
- 1.2. Linear sweep voltammetry, differential pulse voltammetry, square-wave voltammetry, stripping methods-electrode materials, hydrodynamic effects, microelectrodes, and voltammetric sensors.
- 1.3 Determination redox potentials of some inorganic samples.

Unit - II: Analysis of Soil

- 2.1. Analysis of soil: Composition of soil, Concept of pH and pH measurement,
- 2.2 Complexometric titrations, Chelation, Chelating agents, use of indicators
- 2.2. Estimation of Calcium and Magnesium ions as Calcium carbonate by complex ometric titration. (Theory only)

Unit - III: Analysis of Water

- 3.1. Analysis of water: Definition of pure water, sources responsible for contaminating water, water sampling methods, water purification methods.
- 3.2. Dissolved oxygen in water. Determination of dissolved oxygen (DO) of a water sample.
- 3.3 Determination of pH, acidity and alkalinity of a water sample.(Theory only)

Unit - IV: Analysis of Food Products

- 4.1. Analysis of food products: Nutritional value of foods, idea about food processing-food preservations, Methods of food preservations and adulteration.
- 4.2. Identification of adulterants in some common food items like coffee powder, asafoetida, chilli powder, turmeric powder, coriander powder and pulses, etc.
- 4.3 Analysis of preservatives, flavorants, and colouringmatter.(Theory only)

Unit - V: Analysis using Chromatographic Techniques

- 5.1. Chromatography: Definition, general introduction on principles of chromatography,
- 5.2 paper chromatography, TLC-Identification and comparison of samples using TLC method (Organic, inorganic, paints, etc.,)
- 5.3. Separation of compounds using Column (Neutral, acidic and basic columns), ion exchange chromatography.

References

- 1. H. H. Willard, L. L. Merritt, J. Dean, & F. A. Settoe, *Instrumental Methods of Analysis*. 7th Ed. Wadsworth Publishing Co. Ltd., Belmont, California, USA, 1988.
- 2. Douglas A. Skoog,; F. James Holler,; Stanley R. Crouch, *Principles of Instrumental Analysis*, 6thEdition;Cengage Learning, 2006.
- 3. D. A. Skoog, D. M. West, & F. J. Holler, *Fundamentals of Analytical Chemistry*, 6th Ed., Saunders College Publishing, Fort Worth, 1992.
- 4. Harris, D. C. Quantitative Chemical Analysis, W. H. Freeman, 2010.
- 5. Dean, J. A. Analytical Chemistry Notebook, 2nd edition, McGraw Hill, 2004.
- 6. Reuben Alexander Day,; Arthur Louis Underwood, *Quantitative Analysis*, 6thEdition;Prentice Hall India Learning Private Limited, 1992.
- 7. D. Freifelder, *Physical Biochemistry*, 2nd Edition, W.H. Freeman and Co., N.Y. USA, 1982.
- 8. T. G. Cooper, *The Tools of Biochemistry*, John Wiley and Sons, N.Y. USA, 1977.
- 9. Vogel, A. I. Vogel's Qualitative Inorganic Analysis 7th Ed., Prentice Hall, New Delhi, 2009.
- 10. Robinson, J.W. Undergraduate Instrumental Analysis, 5th Ed., Marcel Dekker, Inc., New York, 1995.

)

9 Hours

9 Hours

9 Hours

Semester–V CH550B-Elective-II Protein Chemistry 3 Hrs /week 2 Credits

Objectives

To learn the chemistry of Amino acids and proteins.

To learn the importance of enzymes and enzyme catalysis

Unit - I: Introduction to Proteins

- 1.1 Amino acids-properties and classification of 20 amino acids-Isoelectric point-titration curvepeptide bond-polypeptide-protein-N-ter and C-ter-protein sequence
- 1.2 Primary, secondary-Ramachandran plot-
- 1.3 Tertiary structure Stability of protein structure-protein folding

Unit - II: Purification of Proteins

- 2.1 Separation of proteins-dialysis-column chromatography-ion-exchange chromatographysize-exclusion chromatography-Affinity chromatography,
- 2.2 Electrophoresis-Isoelectric focussing-two-dimensional electrophoresis. Determination of proteins sequence N-terminal amino acid analysis
- 2.3 Sanger's Method-Edman degradation-C-terminal amino acid-carboxypeptidases

Unit - III: Enzymes

- 3.1 Definition-classification of enzymes. Thermodynamics model for enzyme catalysis-Proximity effects-transition state stabilisation-Acid/base catalysis in enzymatic reactions-use of strain energy in enzyme catalysis-
- 3.2 Enzyme Kinetics-Michaelis Menton Equation; Lineweaver-Burk plot-
- 3.3 Factors affecting catalytic activity of enzymes-temperature-pH-concentration. Allosteric enzymes.

Unit - IV: Chemistry of Enzyme Catalysis

- 4.1 Mechanism of chymotrypsin (hydrolytic peptide cleavage)-catalytic triad (nucleophilic addition/hydrolysis) Lysosyme-mechanism-cleavage of peptidoglycans (S_N1/S_N2)
- 4.2 Mechanism of Alcohol dehydrogenase-Oxidation of alcohol (Redox reaction)
- 4.3 Mechanism of Class I fructose-1,6-bisphosphate aldolase (Carbon–Carbon Bond Formation).

Unit -V: Chemistry of Co-Enzymes

- 5.1 The pyridine nucleotide coenzyme-niacin deficiency-the flavin nucleotide coenzyme.
- 5.2 Structure and significance of Thiamine phosphate-
- 5.3 Biotin-pyridoxal phosphate-tetrahydrofolate.

References

- 1. Lehninger, Nelson, Cox, *Biochemistry*, 6th edition, W H Freeman & Co, USA, 2013.
- 2. Berg, Stryer, Tymoczko, *Biochemistry*, 3rd edition, W H Freeman & Co, USA, 2015.
- 3. T. D. H Bugg, *Introduction to enzyme and coenzyme chemistry*, 3rd edition, Wiley-Blackwell, 2012.
- 4. Paula Yurkanis Bruice, Organic chemistry, 6th edition, Pearson Edition, New York, 2006.

Semester - V CH550C-Elective-II Cheminformatics 3 Hrs/week 2 Credits

Objectives

To enable the students to understand the basics of computers

To enable them to operate computers draw chemical structures using some chemistry software's

9 Hours

9 Hours

9 Hours

NAAC 5th CYCLE

9 Hours

To make chemical calculations using computer programs.

Unit – I: Introduction to Chemoinformatics

- **1.1** Definition of Chemoinformatics, History of chemoinformatics, Uses of Chemoinformatics
- 1.2 Representing the molecules: Older systems Connection tables, Line notation INCHI, SMILES, and WLN canolications.
- 1.3. Line notation versus connection tables. Query languages SMARTS. Nomenclature: IUPAC names, trade names, common names. Introduction to chemical structure file formats 2D and 3D

Unit – II: Structure Searching

- 2.1 2D-Fingerprints-Structural Keys Hashed fingerprints, Exact structure searching, Substructure search, Sub similarity search
- 2.2 Ways to measure Similarity 2D topology, 3D configuration. Physical properties, clustering.
- 2.3 Basics of computation of physical and chemical data and structure descriptors, data visualization.

Unit - III: Databases and Packages for chemists

- 3.1 Introduction-Database concepts-**types**-chemical, proteomic, genomic and literature databases-source, content and design, applications.
- 3.2 Chemical databases-Chembank, ChemPDB, Combichem, NCI- Pubchem (Compounds, Substances, Bioassay), PubMed, DrugBank, Chem Spider
- 3.3 ChemDraw, Chem sketch, OriginLab, essential FT IR etc, kinetics. Chemistry free softwares (Argus Lab, Avogadro)

Unit IV: Introduction to drug design:

- 4.1 Target Identification and Validation; Lead Finding and Optimization;
- 4.2 Analysis of HTS data; Virtual Screening; Design of Combinatorial Libraries; Ligand-Based and Structure-Based Drug Design;
- 4.3 Application of Chemoinformatics in Drug Design

Unit V: Practicals

- 5.1 Draw the structure of simple organic molecules-derive name using the softwares-Chemdraw
- 5.2 Building a molecule and energy optimization using ARGUSLAB
- 5.3 Docking of small molecules using ARGUSLAB

Reference Books:

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

2. Larsen et al (ed), Textbook of Drug Design and Discovery, 3rd edition, Taylor and Francis, London and NewYork, 2004.

3. Leach A.R, Molecular Modelling: Principles and applications, 2nd edition, Prentice Hall, New Delhi, 2001.

4. K.V. Raman, Computer Applications in Chemistry, Tata McGraw Hill, New Delhi, 2008.

5. Vikas Gupta, Computer Course Kit, Dream Tech Press, 2010

Web sources:

1. https://open-babel.readthedocs.io/en/latest/Cheminf101/index.html

 $2.\ https://open-babel.readthedocs.io/en/latest/Cheminf101/represent.html#iupac-names-trade-names-common-names$

3. https://open-babel.readthedocs.io/en/latest/Cheminf101/similarity.html

9 Hours

9 Hours

NAAC 5th CYCLE

9 Hours

9 Hours

4. http://insideinformatics.cambridgesoft.com/webinars/info/Default.aspx?webinarID=632

- 5. http://www.acdlabs.com/resources/freeware/chemsketch/
- 6. http://www.acdlabs.com/download/technotes/2016/technote chemsketch advanced.pdf

7. accelrys.com/products/pdf/isis-draw.pdf

8. http://www.originlab.com/doc/Tutorial

9. http://www.inflibnet.ac.in/

10.https://www.khanacademy.org/

Learning Outcomes:

Describe the various methods of representing molecules in a chemical database Explain the fundamentals principles of the various computational methods Chemical calculations using computer programs and docking process were learned.

CH639- Organic Chemistry - V Hrs/week – 4 (Credits 4) **SEM VI Objectives**

Understanding the reactions of bioorganic compounds.

Understanding photochemical reactions.

Learning the structure and reactions of bioorganic and natural molecules.

Unit 1 Carbohydrates

- 1.1 Classification of carbohydrates. D,L notation, configuration of aldoses and ketoses. Reactions of monosaccharides in basic solution, oxidation, reduction reactions.
- 1.2 Osazones, Chain lengthening of aldoses, shortening the chain. Stereochemistry of glucose fishcers proof.
- 1.3 Cyclic hemiacetals of monosaccharides. Glucose the most stable aldohexose, formation of glycosides, anomeric effect, reducing and nonreducing sugars.
- 1.4 Disaccharides and polysaccharides.

Unit 2 Amino acids and catalysis

- 2.1 Amino acids classification, configuration of aminoacids, acid base properties of amino acids, isoelectric point.
- 2.2 Synthesis of amino acids, peptide and disulfide bonds, synthesis of peptide bonds Nprotection and C-activation, determining the primary structure of proteins.
- 2.3 Acid catalysis, base catalysis, nucleophilic catalysis, metal ion catalysis
- 2.4 Intramolecular reactions and catalysis.

Unit 3 Photochemistry

- 3.1 Laws of Photochemical equivalence, primary, secondary processes, quantum yield, light induced reactions, photosensitized reactions, photolysis and flash photolysis.
- 3.2 Photochemical elimination reactions, Norrish I and II, Barton reaction, Photochemical reductions, photochemical oxidations.
- 3.3 Photochemical isomerisations, phantom triplet, photochemical rearrangements.
- 3.4 Photochemical cyclisations and intermolecular cycloadditions.

Unit 4 Natural products I

- 4.1 Alkaloids: isolation, determination of structure of alkaloids (functional nature, estimation of C-methyl, degradation of alkaloids.
- 4.2 Structural elucidation of alkaloids: Adrenaline, piperine, nicotine and cocaine.

12 Hours

12 Hours

12 Hours

4.3 Terpenoids: isolation, general characteristics of terpenoids, determination of structure of terpenoids and monoterpenoids or terpenes.

4.4 Structural elucidation of terpenoids: Myrcene, citral, limonene and menthol.

Unit 5 Natural products II (Natural pigments)

5.1 Carotenoids: isolation and separation, general properties and principal methods in elucidating the constitution of carotenoids, functions and classification of carotenoids.

12 Hours

- 5.2 Carotenes: geometrical isomerism, structural elucidation of carotenes: β -carotene, α -carotene and lycopene.
- 5.3 Fatty acids, waxes, fats and oils are triacylglycerols, phospholipids and spingholipids.
- 5.4 Chemistry of nucleic acids: Nucleosides and nucleotides, composition of nucleic acids.

Reference Books:

Text Books

Paula Yurkanis Bruice, Organic chemistry, 6th Edition, Prentice Hall, Illinois, 2011.

- O. P. Agarwal, Organic Chemistry of Natural Products Vol I & II, Goel Publishing House, New Delhi, 2002.
- 3. P<u>etr Klán, Jakob Wirz</u>, Photochemistry of Organic Compounds: From Concepts to Practice, 1st Edition, Wiley-Blackwell, Chichester, 2001.

Further reading

- 4. R.T. Morrison and R. N. Boyd, *Organic chemistry*, 6th Edition, Prentice-Hall of India, New Delhi, 2008.
- 5. Leroy. G. Wade, *Organic chemistry*, 6th Edition, Pearson, New York, 2005.
- 6. Clayden, J Greeves, N and Warren, S, *Organic Chemistry*, 2nd Edition, Oxford University Press, New York, 2001.
- 7. Loudon, Marc G, Organic Chemistry, 6th Edition, Oxford University Press, New York, 2016.

Outcomes

Knowledge on bioorganic compounds.

Ability to apply reactions and reagents to synthetic aspects of natural products.

SEM VI CH640-Inorganic Chemistry - IV Hrs/week – 4 (Credits 4)

Course Objectives:

To study the chemistry of coordination compounds and organometallic compounds To understand the chemistry of bioinorganic molecules and chemistry of solids.

Unit-1 Coordination Compounds I

- 1.1 Double salts and coordination compounds. Werner's work: primary and secondary valencies.
- 1.2 Sidgwick's theory and Pauling's theory Effective atomic numbers (EAN).
- 1.3 Classification of ligands. IUPAC nomenclature of coordination compounds. Chelates and their uses-stereochemistry of complexes.
- 1.4 Isomerism: Ionization, hydrate, ligand, linkage, coordination, position, geometrical and optical. Methods of detecting complex formation-conductivity and precipitation studies.

Unit-2 Coordination Compounds II

- 2.1 Valence bond theory- hybridization-geometry and magnetic properties-demerits of VBT.
- 2.2 Crystal field theory- crystal field splitting in octahedral, tetragonal, square planar and tetrahedral complexes- CFSE calculation of octahedral complexes.

12 hours

12 hours

- 2.3 Low spin and high spin complexes, spectrochemical series, and explanation of magnetic properties, colour and geometry using CFT. Jahn Teller distortion and *trans* effect.
- 2.4 Labile and inert complexes, thermodynamic stability, kinetic stability, factors affecting the stability of complexes.

Unit-3 Organometallic compounds

12 hours

- 3.1 Metal carbonyls: 18 electron rule, mono and binuclear carbonyls of Ni, Fe, Co and Mn-preparation, structure, chemical properties and uses.
- 3.2 Structure and bonding in π -metal alkenyl, alkynyl and cyclopentadienyl complexes. Olefin organometallics: preparation and uses. Allyl organometallics: preparation and uses.
- 3.3 Cyclopentadienyl organometallics: preparation and reactions.
- 3.4 Synthetic applications of organometallic compounds as homogenous catalyst-Wilkinson catalyst, Fischer-Tropsch reaction.

Unit-4: Bioinorganic Chemistry

- 4.1 Porphyrin ring systems: cytochromes, structure and functions of Haemoglobin and Myoglobin.
- 4.2 Chlorophyll: structure, functions and Photosynthesis. Structure and functions of Vitamin B₁₂.
- 4.3 Biochemistry of Iron. Metalloenzymes- Carboxypeptidase and Carbonic anhydrase.
- 4.4 Biological fixation of Nitrogen and Nitrogen cycle.

Unit-5 Chemistry of solids

- 5.1 Crystalline and amorphous solids-Definition and differences. Symmetry in solid crystals-Basic crystal systems with example to each system.
- 5.2 Structure of solids- close packing of spheres- Primitive cube-BCC-FCC- Radius ratio rule.
- 5.3 Types of crystals-ionic-covalent-metallic and molecular crystal with one example. and shape of ionic crystals (AB= NaCl, $AB_2 = CaF_2$).
- 5.4 Defects in solids-stoichiometric defects (Schottky, Frenkel) and nonstoichiometric defects (metal excess and metal deficiency).

Learning Outcomes

Explain the basics and advance concepts of coordination compounds

Explain the bonding and isomerism in coordination compounds

Outline the different organometallic compounds and explain their synthetic applications.

Explain the basics of bioinorganic chemistry and solid states

References

(Text Book)

- 1. R. D. Madan, *Modern Inorganic Chemistry*, Second edition, S. Chand publications, New Delhi, 2000.
- 2. B. R. Puri, L. R. Sharma and K. C. Kalia, *Principles of Inorganic Chemistry*, 33rd Edition, Vishal Publishing Co, Jalandar, 2004.
- 3. 1. J. D. Lee, *Concise Inorganic Chemistry*, Chapman and Hall: London, 1961.
- 4. R. Gopalan and V. Ramalingam, *Concise Coordination Chemistry*, First Edition, S.Chand (G/L) & Company, 2001

(Advanced Reading)

- 1. C. Chambers and A. K. Holliday, *Modern Inorganic Chemistry*, First edition, Butterworth and Co., Sussex, 1975.
- 2. Gary L Miessler and Donald A. Tarr, *Inorganic Chemistry*, Third edition, Pearson Prentice Hall.

- prentice Hall, New York, 2008.G. A. Lawrence, *Introduction to Coordination Chemistry*, Wiley, 2009
 - 5. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, Fourth Edition. Wiley-Interscience Publication, US, 1980.

3. A. G. Sharpe and C. E. Housecraft, *Inorganic Chemistry* Vol-I, 3rd edition, Pearson

SEM VI CH641-Physical Chemistry - IV Hrs/week – 4 (Credits 4) Objectives

- To know the fundamentals theories that govern the electrolytic conductance in solids and solutions and apply them to solve problems related to it.
- To learn about the acids and base equilibria
- To know about the different types of electrochemical cells and their importance

Unit - I: Ionic Equilibria -I

- 1.1 Electrolytic conduction: conductor non-conductor types of conductors-Electrolytic and metallic conductors.
- 1.2 Specific conductance, equivalent conductance and molar conductance measurement of these quantities Variation of equivalent conductance with dilution.
- 1.3 Arrhenius theory of Ionization (and Limitations of the theory)-Factors governing degree of dissociation of an electrolyte-Ostwald Dilution Law*-(Limitation of Ostwald's Law-Factors that explain the failure of Ostwald's law in case of strong electrolytes) -
- 1.4 Kohlraush'slaw and its applications. Debye Huckel theory of strong electrolytes Onsagar equation (No derivation) significance and limitations.

Unit - II: Ionic Equilibria -II

- 2.1 Migration of ions –ionic mobility and its determination. Transport number and its determination by Hittorf and moving boundary methods.
- 2.2 Applications of conductance measurements: Determination of degree of dissociation of weak electrolytes, ionic product of water, solubility of sparingly soluble salts.
- 2.3 Conduct metric titrations: Strong acid strong base, weak acid strong base, Strong acid weak base, mixture of strong acid and weak acid strong base, Precipitation titration.
- 2.4 pH and pOH: Definition and explanation. Calculation of weak acids and base

12 Hours

Unit - III: Ionic Equilibria-III

- 3.2 Solubility product and its relationship to solubility. Application in qualitative analysis
- Common ion effect applications in analysis. 3.3
- Hydrolysis of salts: Expression for hydrolysis constants, degree of hydrolysis and pH of 3.4 salt solution, strong acid and weak base, weak acid strong base, weak acid and weak base.

Unit - IV: Electromotive Forces

- Electromotive force: Galvanic cells reversible and irreversible cells Daniel cell -4.1 EMF of the cell and its determination by potentiometric method. Standard cell (Weston cadmium cell).
- 4.2 Reversible electrodes -representation, construction and reaction of metal -metal ion electrode, gas electrode (hydrogen, oxygen, chlorine), calomel electrode, single electrode potential and its determination.
- 4.3 Derivation of Nernst equation for EMF of the cell and single electrode potential. Standard electrode potential, sign and convention.
- 4.4 Electrochemical series and its significance. Derivation of relationship between thermodynamic quantities ΔG , ΔH , ΔS , and cell EMF.

Unit - V: Applications of EMF

12 Hours

- 5.1 Chemical cell with and without transport. Concentration cells with and without transport. Expressions for EMF-Liquid junction potential
- 5.2 Application of EMF measurements: Determination of activity coefficient, transport number, valence of doubtful ions, solubility of sparingly soluble salts and equilibrium constant.
- 5.3 Determination of P^{H} using hydrogen electrode, quinhydrone electrode and glass electrode. Potentiometric titrations. (Acid base titration, precipitation titration and redox titration).
- . 5.4 Fuel cells. Storage cells- Lead storage battery and Lithium-ion battery Li polymer battery.

Text Books:

- 1. B. R. Puri, L. R. Sharma and M. S. Pathania, Principles of Physical Chemistry, 47th Edition, Vishal Publishing Co, Jalandar, 2016.
- 2. R.L. Madan, *Physical Chemistry*, Mc Graw Hill Education Pvt. Ltd. 2015.

Reference:

- 1. Arun Bahl, B.S. Bahl. G.D.Tuli, Essentials of Physical Chemistry, S. Chand Publications
- 2. A.S. Negi and S.C. Anand, A text book of Physical Chemistry, Wiley Eastern Ltd, New Delhi, 1984.

Learning Outcome

Discuss the fundamental and important aspects of chemical and ionic equilibrium Predict the electrochemical properties of a cell reaction.

Subject Skill

NAAC 5th CYCLE

Semester - VI

Objectives

- To understand the mechanism of polymerization, various techniques of polymerization
- To learn about the characterization of polymers by molecular weight, reactions and degradation of polymers.
- To learn the applications and appreciate the recent developments of polymers.

Polymer Chemistry

15 Hours Unit - I: Introduction to Polymers and Mechanism of Polymerization

- Polymer: introduction, classification of polymers: natural, synthetic, organic, inorganic, 1.1 elastomers, fibers, resins, and plastics: thermoplastic and thermosetting.
- Copolymers and its types. Types of Polymerisation methods 1.2
- 1.3 Addition- radical and ionic polymerization, Coordination polymerization.
- Step polymerization-poly condensation, poly addition and ring opening. 1.4
- Miscellaneous polymerization reactions: electrochemical, metathetical, 1.5

Unit - II: Molecular Weight, Structure and Properties of Polymers

- 2.1 Molecular weight of polymers: number average, weight average, sedimentation and viscosity average molecular weight, degree of polymerization and practical significance of polymer molecular weight with problem solving
- Molecular weight determination methods: ultracentrifugation and viscometry. 2.2
- Physical properties of Polymers: Mechanical properties (Impact resistance, Tensile 2.3 strength and Melt viscocity)-Tacticity- nature of chain packing-Chain flexibility.
- 2.4 Glass transition temperature-Factors affecting Tg- Molecular weight and Tg-Plasticisers and Tg- Importances of Tg.
- 2.5 Reactions-Hydrolysis, Hydrogenation, addition, substitution, cross linking, vulcanization and cyclisation.

Unit - III: Polymerisation Techniques and Polymer Processing

- Polymerisation techniques: Bulk, solution, suspension and emulsion polymerization -3.1 melt polycondensation.
- 3.2 Polymer processing- Calendaring -Casting methods: Die casting, rotational casting and Film casting.
- 3.3 Moulding techniques-Compression, Injection, Blow and Extrusion Moulding.
- Thermoforming-Foaming- Reinforcing (hand Lay-up, Filament winding and Spray-up 3.4 Techniques).
- 3.5 Fibre spinning methods: (Melt spinning-Dry spinning and Wet spinning)

Unit - IV: Commercial Polymers

- 4.1 Preparation, properties and uses of the following: Polyethylene, Polystyrene, TEFLON and PVC.
- 4.2 Preparation, properties and uses of the following: -Polyesters, Polyamides, Polycarbonates Polyurethanes, Polypropylene Glycols (PPG).
- Preparation of Epoxy resins, Styrene butyl rubber, Rayon and Carboxy Methyl 4.3 cellulose.
- 4.4 Polymer additives: Fillers (Wood, Flour, Asbestos, Graphite and Mica), Plasticizers (Tricresyl phosphate, Dimethyl Phthalate and Camphor)- Structure and uses
- 4.5 Fire Retardants Pyro Check 68PB and Halogen free fire retarding plastics and Colourants.

Unit -V: Introduction to Recent Trends in Polymer

CRITERION I

NAAC 5th CYCLE

15 Hours

5 Hrs/week (4 Credits)

15 Hours

15 Hours

- 5.1 Biodegradable polymers: Polyhydroxyalkonates (Biodegradation and application), Poly Lactic acid (synthesis and application), Aliphatic and aromatic polyesters (Degradation)-.
- 5.2 Conducting Polymers: Ionic conduction in solid electrolyte systems, Electronic conducting materials in non – conducting polymers
- Electronically conducting polymer Poly sulphur nitride, Polyacetylene and Poly 5.3 phenylene.
- 5.4 Polymers as Biomaterials: artificial heart, Artificial skin, contact lenses, Artificial kidneys.
- Inorganic Polymers: Preparation and properties of Silicones, Phosphonitriles. 5.5

References

- 1. F.W. Bill Meyer, Text Book of polymer science, Wiley & Sons, 1984.
- 2. Gowariker. V.R. Viswanathan, N.V. Jayader Sreedhar. Polymer, Wiley Eastern Ltd., New Delhi, 1978.
- 3. B.K. Sharma, *Polymer Chemistry*, Goel Publishing house, Meerut, 1989.
- 4. Polymer Chemistry by M.K. Mishra, New Age Publications, New Delhi.
- 5. M.G.Arora, M.S.Vadar, Polymer Chemistry. Anmol publication (p) Ltd., New Delhi, 1989.
- 6. Jagadamba Singh and R.C.Dubey, Organic Polymer chemistry- Pragati Publishers Meerut, 2012.

Semester - VI Industrial and Environment Chemistry 5 Hrs/week (4 Credits) **Objectives:**

To introduce the students about industrial extraction processes.

The pollution induced by the industrial development and the care towards the environment is focused.

Unit - I: Chemical Technology

- 1.1. Basic principles of distillation, solvent extraction, methods of leaching separation by absorption and adsorption.
- 1.2. An introduction into the scope of different types of equipment needed in chemical technology, including chemical reactors, distillation columns, extruders, pumps, mills,
- 1.3. Scaling up operations in chemical industry. Problems involving the scaling up of the process. Scale up and process development-Scale up and modeling
- 1.4. Introduction to clean technology for speciality chemicals-economic, environment and safety needs. Clean technology route to waste management

Unit - II: Industrial Metallurgy

- 2.1. General Principles of Metallurgy
- 2.2. Hydrometallurgy, Methods of purification of metals Al, Pb, Ti, Fe, Cu, Ni, Zn.
- Refining of metal electrolytic, oxidative refining, Kroll process, Parting process, van 2.3 Arkel-de Boer process and Mond's process.
- 2.4 Ultrapure metals for semiconductor technology and their applications.
- 2.5. Alloys Composition and its importance.

Unit - III: Eco systems and Air Pollution

- 3.1. Ecosystems. Biogeochemical cycles of carbon, nitrogen and sulphur.
- 3.2. Air Pollution: Major regions of atmosphere. Chemical and photochemical reactions in atmosphere. Air pollutants: types, sources, particulate size and chemical nature;
- 3.3 Photochemical smog: its constituents and photochemistry. Environmental effects of ozone, Major sources of air pollution.

15 Hours

15 Hours

15 Hours

NAAC 5th CYCLE

- 3.4. Pollution by SO₂, CO₂, CO, NO_x, H₂S and other foul smelling gases. Effects of air pollution on living organisms and vegetation.
- 3.5. Greenhouse effect and Global warming, Ozone depletion by oxides of nitrogen, chlorofluorocarbons and Halogens, removal of sulphur from coal.

Unit - IV: Aquatic Ecosystems and Purification Systems

- 4.1. Water Pollution: Hydrological cycle, water resources, aquatic ecosystems, Sources and nature of water pollutants, Techniques for measuring water pollution, Impacts of water pollution on hydrological and ecosystems.
- 4.2. Water purification methods. Effluent treatment plants (primary, secondary and tertiary treatment).
- 4.3 Industrial effluents from the following industries and their treatment: electroplating, textile, tannery.
- 4.4. Industrial waste management, incineration of waste. Water treatment and purification (reverse osmosis, electro dialysis, ion exchange).
- 4.5. Water quality parameters for waste water, industrial water and domestic water.

Unit - V: Energy & Environment

- 5.1. Classification renewable and non-renewable. Sources of energy: Coal, petrol and natural gas. Uses and its impact on environment.
- 5.2. Nuclear Fusion/Fission. Process, its uses and its environmental impacts to aquatic life.
- 5.3. Nuclear Pollution: Disposal of nuclear waste, nuclear disaster and its management.
- 5.4. Clean energy: Solar energy, Wind Energy, Hydrogen, geothermal, Tidal and Hydraulic energy, etc.
- 5.5. Fuel cells, bio mass, biogas preparation and its environmental impacts

Books for Reference

Semester -VI

- 1. E. Stocchi: Industrial Chemistry, Vol-I, Ellis Horwood Ltd. UK. 1990.
- 2. R.M. Felder, R.W. Rousseau: Elementary Principles of Chemical Processes, Wiley Publishers, New Delhi, 2015
- 3. K. De, Environmental Chemistry, New Age International Pvt., Ltd, New Delhi, 2006
- 4. S. M. Khopkar, Environmental Pollution Analysis: Wiley Eastern Ltd, New Delhi, 2007
- 5. W. Hoyle, Clean Technology for the Manufacture of Speciality Chemicals, Royal Society of Chemistry, Manchester, UK, 2001

Subject Skill Green Chemistry

Objectives To understand the environmental concern and shrinking resources

To learn the environmentally friendly products and procedure.

To take a natural view of different chemical processes

Unit - I: Introduction to Green Chemistry

- 1.1 Introduction to Green chemistry- What is Green chemistry- Need for green chemistry
- Explanation of the twelve Principles of green chemistry 1.2
- 1.3 Planning a green synthesis in a chemical laboratory- percentage atom utilization, evaluating the type of the reaction involved, selection of appropriate solvent, starting materials, use of protecting group, catalyst, microwaves and sonication
- 1.4 Atom economy- synthesis of Ibuprofen. Solvent free reactions- scope, utility of solvent free conditions and controlling solvent free reactions.

Unit - II: Green Synthesis - I

15 Hours

15 hours

15 Hours

5 Hrs / week (4 Credits)

- 2.1 Organic synthesis in water as Green solvents-pericyclic reaction, Claisen rearrangement, wittig- horner reaction, Aldol condensation, pinacol coupling
- 2.2 Oxidation, Reduction, Electrochemical synthesis, Carbon- carbon bond formation in aqueous medium (H_20)
- Organic synthesis in supercritical carbon dioxide(SC- CO₂)- properties, phase diagram, 2.3 as dry cleaning, solvent for organic reaction, asymmetric catalyst, SC polymerization, free radical bromination, Kolbe schmitt reaction
- 2.4 Hydroformylation, hydrogenation, oxidation, coupling reaction, photochemical reaction and biotransformation in SC- CO2. Formation of silica nano particles using SC- CO2.

Unit - III: Green Synthesis - II

- 3.1 Green synthesis compounds like adipic acid, alcohols, cyclohexane oxime, progesterone, paracetamol and polyaspartates
- 3.2 Using Green catalysts - Phase Transfer catalyst- mechanism, types, advantages and applications. Cobalt carbonyl catalysed carbonylation, esterification by PTC.
- Comparison of heterogeneous and homogenous catalysis, bio catalysis, asymmetric and 3.3 photo catalysis. Photolysis of benzophenone, olefins, free radicals and Barton reactions
- 3.4 Dye removal- Chemical methods- oxidative processes using fentons reagent, NaOCl and Electrochemicalprocess. Physical methods and Biological treatments

Unit - IV: Green Synthesis - III

- Microwave assisted organic synthesis- Hydrolysis of benzyl chlorides, benzamide, 4.1 benzoic acid and N-phenyl benzamide. Oxidation of toluene, Coupling of amines with halides and Heterocyclisation
- 4.2 Ultrasound assisted organic synthesis- Instrumentation, types of sonochemical reactions- organometallic reactions, saponification and alkylation. Sonolysis of Fe(CO)5.
- 4.3 Organic synthesis using polymer supported catalystsphotosensitizers, metalloporphyrin, super acid catalyst and crown ethers
- 4.4 Organic synthesis using Ionic liquids and solids- Knoevenagel reactions, Michael reactions, Wittig reactions and Grignard reaction

Unit - V: Future of Green Chemistry

- Future trends in green chemistry-designing next generation agrochemicals from natures-5.1 biopesticides approach, classical, innundative approach and its limitation of biological control.
- Source of biorational pesticides- allelopathy and microbials. Botanicals as source of 5.2 agrochemicals. Isolation and identification of the natural products
- Organic synthesis using green reagents- ozone, H2O2, dioxiranes, peroxy acids, 5.3 dimethylcarbonates and polymer supported reagents.
- Organic synthesis using biocatalysts- biochemical oxidation, biochemical reduction and 5.4 enzymes catalysed hydrolytic processes

References

- V. K. Ahluwalia, A textbook *Green chemistry*, published by N. K. Mehra, Narosa Publishers., 2013
- Rashmi sanghi & M M Srivastava, Green chemistry, Environmental friendly alternatives, Alpha Science International, 2003
- M. A. Ryan & Tinnesand, Introduction to Green chemistry, Amerian chemical society, Washington, 2002.
- 4. A. S. Matlack, Introduction to Green Chemistry, Mercel Deckkar, 2001.
- 5. M. C. Cann & M. E. Connely, *Real world in green chemistry*, ASC, Washington, 2000.

15 Hours

NAAC 5th CYCLE

15 Hours

- 6. P. T. Anastas & J. K. Warners, Green chemistry- Theory and practical, Oxford University press, 1998.
- 7. V.K Ahluwalia, Green chemistry, Environmentally benign reactions, 2009

Subject Skill Materials Chemistry

- To understand the basic concepts of crystal structures and their characterization
- To learn about different properties of solid state materials and their characteristic structural features

Unit - I: Solid State

Semester - VI

Objectives

- 1.1 Structure of solids- close packing of spheres- Primitive cube-BCC-FCC- structure type AX-NaCl.
- 1.2 Types of cubic systems- simple, BCC and FCC.
- 1.3 Metallic Bond-Electron gas and band theories.
- 1.4 Defects in solids-stoichiometric and non-stoichiometric defects.
- 1.5 X-ray Diffraction-Principle-Bragg's equation.

Unit - II: Analysis of Solid States

- 2.1 Neutron diffraction Principle-Comparison of X-ray and Neutron Diffraction.
- 2.2 Structure of AX₂-CaF₂, Rutile, CdI₂, nickel arsenide
- Structure of perovskite and spinels 2.3
- Electrical, Magnetic and optical properties of solids, semiconductors, superconductors, 2.4
- 2.5 Solid-state Electrolytes-Semiconductors and Super conductors - BCS theory

Unit - III: Magnetic Properties

- 3.1 Magnetic dipole moment- Magnetization-magnetic flux density-magnetic permeability, susceptibility.
- 3.2 Types of magnetic behavior: Dia, para, ferro, antiferro and ferrrimagnetism: Hysterisis.
- Pyroelectricity-piezo electricity- relationship between ferro, piezo and pyroelectricity. 3.3
- 3.4 Reactions of solid state and phase transitions, Diffusion, Diffusion coefficient, Diffusion mechanisms, Vacancy and interstitial diffusion, Formation of Spinel's.
- 3.5 Solid state lasers, inorganic phosphors, Ferrites, Garnets.

Unit - IV: Nanomaterials

- Nanomaterials-Size dependent properties- melting points, magnetism, colors, 4.1 conductivity-applications of nanometals-colors-catalysis, electronics
- Synthesis of nanometals- gas phase and chemical synthesis. 4.2
- Semiconductor nanocrystals, quantum dot conductors, syntheses-CdTe, CdS-spherical 4.3 and triangular nanocrystals.
- Introduction-topical areas-pharmacy, therapeutic drugs, ceramics, insulators, metals, 4.4 environmental chemistry, catalysts, polymers, paints, batteries.
- Size relationships of chemistry, nanoparticles and condensed matter-classification of 4.5 nanomaterials.

Unit - V: Nanocrystals

- 5.1 Ceramic nanocrystals-synthesis-physical methods-vapor condensation, spray pyrolysis
- Chemical methods-sol-gel technique, reverse micro emulsions/micelles method, 5.2 Mechano-chemical synthesis
- Chemical and physical properties. Chemical and catalytic aspects of nanocrystals 5.3
- Catalytic properties of metals-metal oxides, sulfides and halides, 5.4
- Nanostructured adsorbents-nanoparticles as new chemical reagents. 5.5

15 Hours

15 Hours

15 Hours

15 Hours

15 Hours

5 Hrs / week (4 Credits)

References

- 1. A. R. West, Basic Solid state chemistry, John Wiley, 1991.
- 2. W. E. Addison, Structural Principle in inorganic chemistry, Longman, 1961.
- 3. D.M. Adams, *Inorganic solids*, John Wiley Sons, 1974.
- 4. C. N. R. Rao, Advances in Solid State Chemistry, Cambridge University Press, 1997
- 5. Guozhong Cao, *Nanostructures & Nanomaterials Synthesis, Properties & Applications*, Imperial College Press, 2004
- 6. T.Pradeep, *Nano: The Essentials*, Mcgraw-Hill Professional, 2008.
- 7. V.Rajendran Materials Science, McGraw Hill Education, 2011.
- 8. M.Arumugam, Materials Science, Anuradha Publications, Chennai, 2016.

Semester-VI Water Chemistry and Inorganic Materials of Industrial Importance 5 Hrs/Week (4 Credits)

Objectives

- To learn the principles of Water Chemistry and industrial water treatment process
- To understand the principles and properties of Inorganic materials of Industrial importance.
- To study the significance and its applications of Inorganic materials of Industrial importance.

Unit - I: Water Chemistry-I

- Introduction- Origins and scope of water chemistry- Physico-chemical Characteristics of Natural Waters- water quality- Organic load- Chemical parameters governing water quality-
- Classification of water quality- Examples of surface water quality in India Waters of Hydration-Hydrogen Bonding-Free and clustered water.
- 1.3 Common concentration units used in water analysis- chemical concentration units-Interconversion among common and chemical concentration units- Alkalinity and Hardness
- 1.4 Properties of Water at High Temperatures and Pressures- Thermo physical and thermochemical- Properties of water below and above 100°C- Effects of temperature on the ion product of water.
- 1.5 Material Compatibility and Corrosion- Corrosion in aqueous systems- Deposit formation vs. Role of zeta potential- Role of alkalinity in steam-water circuits- Deoxygenation

Unit -II: Water Chemistry-II

- 2.1 Treatment of Natural Waters for Industrial Cooling- Bio fouling in natural waters-Operational practice of chlorination
- 2.2 Materials in a cooling water circuit Ferrous sulphate injection- Cooling water treatment
- 2.3 Demineralization by Ion Exchange- Ion exchange resins-Ion exchange process-Properties of ion exchange resins
- 2.4 Demineralization of natural waters- Quality of DM water
- 2.5 Water side corrosion and deposition problems- Chemical treatment of water for industrial and power plant boilers

Unit - III: Silicate and Ceramics

3.1 *Glass*: Glassy state and its properties, classification (silicate and non-silicate glasses).

15 Hours

15 Hours

Semester-VI

CRITERION I

- Manufacture and processing of glass. 3.2
- Composition and properties of the following types of glasses: Soda lime glass, lead 3.3 glass, armoured glass, safety glass, borosilicate glass, fluorosilicate, coloured glass, photosensitive glass.
- *Ceramics*: Important clays and feldspar, ceramic, their types and manufacture. 3.4
- 3.5 High technology ceramics and their applications, superconducting and semiconducting oxides. Composites: fullerenes, carbon nanotubes and carbon fibre.

Unit - IV Cements and Fertilizers

- 4.1 Cements: Classification of cement, ingredients and their role. 4.2 Manufacture of cement and the setting process, quick setting cements.
- 4.3 Fertilizers: Ammonia Synthesis: Haber's process and Contact Process: Sulphuric acid Nitric acids.
- 4.4 Different types of fertilizers. Manufacture of the following fertilizers: Urea, ammonium nitrate, calcium ammonium nitrate, ammonium phosphates;
- Manufacture of the following fertilizers: polyphosphate, superphosphate, compound 4.5 and mixed fertilizers, potassium chloride, potassium sulphate.

Unit - V: Surface Coatings and Batteries

- **15 Hours** Surface Coatings: Objectives of coatings surfaces, preliminary treatment of surface, 5.1 classification of surface coatings. Paints and pigments-formulation, composition and related properties.
- 5.2 Oil paint, Vehicle, modified oils, Pigments, toners and lakes pigments, Fillers, Thinners, Enamels, emulsifying agents. Special paints (Heat retardant, Fire retardant, Eco-friendly paint, Plastic paint),
- 5.3 Dyes, Wax polishing, Water and Oil paints, additives, Metallic coatings, metal spraying and anodizing.
- 5.4 Batteries: Primary and secondary batteries, battery components and their role.
- Characteristics of Battery. Working of following batteries: Pb acid, Li-Battery, Solid 5.5 state electrolyte battery. Fuel cells, Solar cell and polymer cell.

References

K.S. Venkateswarlu, Water Chemistry-Industrial and Power Station Water Treatment, New Age International (P) Limited, Publishers, 1996.

Patrick Brezonik, William Arnold, Water Chemistry: An Introduction to the Chemistry of Natural and Engineered Aquatic Systems, Oxford University Press, USA, 2011

- 2. R. M. Felder, R. W. Rousseau: Elementary Principles of Chemical Processes, Wiley Publishers, New Delhi, 2015.
- 3. W. D. Kingery, H. K. Bowen, D. R. Uhlmann: Introduction to Ceramics, Wiley Publishers, New Delhi, 2007.
- 4. J. A. Kent: Riegel's Handbook of Industrial Chemistry, CBS Publishers, New Delhi, 2010.
- 5. P. C. Jain & M. Jain: Engineering Chemistry, Dhanpat Rai& Sons, Delhi, 1998.
- 6. R. Gopalan, D. Venkappayya, S. Nagarajan: *Engineering Chemistry*, 4th edition, Vikas Publications, New Delhi, 2013.
- 7. B. K. Sharma: Engineering Chemistry, Goel Publishing House, Meerut, 1998.

Title: Chemistry of Drug Design

Objectives: Introduce the basic concepts of drug design and discovery process Learn the techniques of SAR/QSAR Introduce the concepts of molecular modeling

NAAC 5th CYCLE

5 Hrs/Week (4 Credits)

Introduce the concepts of receptor inhibition and enzyme inhibition in drug design

Unit -I An introduction to drugs, their action and discovery

- Drugs-discovery and design: a historical outline-Leads and analogues-therapeutic index 1.1
- Sources of leads and drugs-Leads and analogues: some desirable properties Introduction 1.2 to drug action-Potency-Selectivity-
- ADME (Absorption, Distribution, Metabolismand Excretion)-Classification of drugs 1.3
- Drug structure and Solubility-Stereochemistry and drug design-Solubility-The 1.4 importance of water solubility
- Partition determination of partition coefficients (Practical /Theoretical) 1.5

Unit II Structure-activity and quantitative structure relationships 15 hours

- 2.1 Structure-activity relationship (SAR/QSAR)-Changing size and shape (Changing the number of methylene groups in chains and rings-increasing or decreasing the degree of unsaturation-introducing or removing a ring system).
- Introduction of new substituents (methyl/hydroxy/halogen/basic/Carboxylic and 2.2 sulphonic acid groups/thiols, sulphides and other sulphur groups), Changing the existing substituents of a lead
- QSAR- (Case study: a SAR investigation to discover potent geminal bisphosphonates) 2.3
- 2.4 Descriptors*-The lipophilic parameters-Electronic parameters- Steric parameters
- Deriving a QSAR equation-simple and multiple linear regression (The Squared 2.5 Correlation Coefficient, R², Cross-Validation).*

Unit III: Computer Aided Drug Design

- Introduction Models Molecular modelling methods-Molecular mechanics-force field 3.1
- Molecular dynamics Docking De novo design Pharmacophores and some of their uses 3.2
- Modelling protein structures-Homology Modeling-web servers for protein modeling 3.3
- 2D-QSAR-Descriptors-Types of Descriptor-Regression Analysis 3.4
- 3D QSAR-CoMFA-Advantages and disadvantages 3.5

Unit IV: Receptors and messenger

- The chemical nature of the binding of ligands to receptors-Structure and classification 4.1 of receptors-
- 4.2 General mode of operation (Superfamily Type 1,2,3,4)-Ligand–response relationships (Experimental determination of ligand concentration-response curves: Agonist concentration-response relationships, Antagonist concentration-receptor relationships, Partial agonists, Desensitisation)
- 4.3 Ligand-receptor theories (Clark's occupancy theory, The rate theory, The two-state model)
- 4.4 Drug action and design Agonists, Antagonists
- Citalopram, an antagonist antidepressant discovered by a rational approach, β -Blockers 4.5

Unit V: Enzymes

- Active sites and catalytic action Allosteric activation 5.1
- 5.2 Regulation of enzyme activity (Covalent modification, Allosteric control, Proenzyme control)
- Enzyme inhibitors-Reversible inhibitors Irreversible inhibition, Transition state 5.3 inhibitors.
- 5.4 Enzymes and drug design-some general considerations Examples of drugs used as enzyme inhibitors (Sulphonamides, Captopril, Statins)

15 hours

15 hours

15 hours

15 hours

5.5 Enzymes and drug resistance (Changes in enzyme concentration, An increase in the production of the substrate, Changes in the structure of the enzyme, The use of an alternative metabolic pathway)

Main Text:

- 1. Medicinal Chemistry (2nd Edition) by Gareth Thomas, John Wiley and Sons Ltd.
- 2. *Chemoinformatics by Andrew R. Leach and V.J. Gillet, Springer

Self Study Paper-IISemester - VIChemistry for Competitive Examinations – II1 CreditObjectives

To motivate the students for self study

To prepare them for the competitive exams

Unit - I: Oxidation and Reduction

Oxidation number-oxidizing and reducing agents-balancing redox equations

Unit - II: Concentration Units

Normality- acid base reactions-Normality-redox reactions-mole fraction and molality.

Unit - III: Thermodynamics

Heat-internal energy-enthalpy, free energy change and entropy.

Unit - IV: Chemical Kinetics

Rate laws-order-molecularity-half life-collision theory.

Unit - V: Electrochemistry

Electrical units-electrolysis-galvanic cells-Nernst equation.

References

- 1. R.L. Madan & G.D Tuli, *Physical chemistry*, Questions and answers, S. Chand success guides, 2012.
- 2. Pearson, *Super course in physical Chemistry*, Dorling Kindersley, 1st edition, 2004.
- 3. Estelle K Meislich, *3000 problems in organic chemistry vol 1 & 2*, Tata McGraw Hill, 2004.
- 4. Mc Graw Hill education series, Complete Chemistry, JEE Main, 2014.

Chemistry Lab Work – III PCH621-Gravimetric Estimations and Organic Analysis

Semester - V & VI

3 Hrs/week (3 Credits/semester)

Objectives

- To acquire sound practical knowledge in the gravimetric estimations.
- To prepare the students for analysing various organic compounds through systematic analysis.
- To enable the student to understand the principles behind the preparations of different organic compounds.

Gravimetric Estimations

Estimation of water of crystallization of hydrated Barium chloride Estimation of Barium as Barium sulphate Estimation of Sulphate as Barium sulphate Estimation of Barium as Barium chromate Estimation of Lead as Lead chromate Estimation of Calcium as Calcium oxalate monohydrate

Organic Analysis

Analysis of organic compounds containing one functional group and characterization with a derivative.

Reactions of the following functional groups:

Aromatic aldehydes, ketones, Aromatic carboxylic acids, esters, carbohydrates, phenols, aromatic primary amines, amides, nitro compounds and anilides.

Organic Preparations

Acetylation:

Acetanilide from aniline

(or)

Aspirin from salicylic acid

Benzovlation:

Benzanilide from aniline

(or) 2-Naphthyl Benzoate from 2-Naphthol

Bromination:

p-Bromoacetanilide from acetanilide

(or)

2.4.6-Tribromoaniline from aniline

Oxidation:

Benzoic acid from benzaldehyde (or)

Benzoic acid from Toluene

Nitration:

m-dinitrobenzene from nitrobenzene

(or)

Picric acid from phenol

Hydrolysis:

a) Benzoic acid from ethylbenzoate

(or)

b) Salicylic acid from methyl salicylate

References

1. Arthur I. Vogel, A Textbook of Practical Organic Chemistry, 4th Edition. ELBS, 1986.

- 2. N.S. Gnanapragasam and B. Ramamoorthy, *Organic Chemistry Lab Manual*, S. Visvanathan Printers & Publishers, 2006.
- 3. A.O, Thomas. *Practical Chemistry*, 6th Revised Edition, Sharada Press, 1995.
- 4. J. N. Gurtu And R. Kapoor, Advanced Experimental Chemistry, Vol. I Physical Chemistry, Vol. II Inorganic Chemistry, Vol. III Organic Chemistry, Organic Reactions & Reagents [B.Sc., (Hons.)& M.Sc.], Himalaya Publications, 1974.

Chemistry Lab Work - IV PCH622-Physical Chemistry Experiments 3 Hrs/week (3 Credits/semester)

Semester - V & VI

Objectives

To understand about physical behaviour of compounds.

To impart sound practical knowledge in understanding the reaction pathways and calculations involved in them.

Phenol - Water system

Determination of Transition temperature of hydrated salts

Determination of molecular weight of a solute - Rast method

Determination of rate constant of acid catalysed ester hydrolysis

Determination of rate constant of inversion of sucrose-polarimetry

Determination of distribution coefficient of iodine between water and CCl₄ (or)benzoic acid between water and benzene

Determination of λ_{∞} of a strong electrolyte

Determination of dissociation constant of a weak electrolyte

Phase Diagram

Measurement of Viscosity

Conductometric titration (strong acid and strong base)

Flame photo meter (Estimation of Na, K, Li)

Potentiometric titration (Redox titration)

pH Meter (strong acid and strong base)

Colorimeter- Determination of concentration of given solution

References

- 1. V. Venkateswaran, R. Veerasamy, A.R. Kulandaisamy, *Basic principles of Practical Chemistry*, S.Chand publications, New Delhi, 2002.
- J. N. Gurtu And R. Kapoor, Advanced Experimental Chemistry, Vol. I Physical Chemistry, Vol. II Inorganic Chemistry, Vol. III Organic Chemistry, Organic Reactions & Reagents [B.Sc., (Hons.)& M.Sc.], Himalaya Publications, 1974.
- 3. V. D. Athavale and Parul Mathur, *Experimental Physical Chemistry*, 1st Edition., New Age Publishers, 2008.
- 4. R. C. Das, *Experimental Physical Chemistry*, Tata McGraw-Hill Publications, 1986.
- 5. S. Giri, D. N. Pandey, O. P Pandey, Pratical Chemistry, S.Chand& Company, 1998.

Non-Major Elective – I

Semester – V NCH504-Chemistry of Drugs & Diseases 2 Hrs / week (2 Credits) Objectives

To learn the basic scientific facts about common drugs.

To understand about different types of diseases and their treatments for a healthy living.

Unit - I: Drug Administration and Blood

- 1.1 Terminology in Pharmaceutical chemistry Pharmacology, Pharmaceutics, toxicology, pharmacopoeia, pharmacy, mutation. Modes of administration of drugs-Enteral routes: oral, buccal and rectal.
- 1.2 Parenteral routes: intradermal, subcutaneous, intramuscular, intravenous, intramedullary, inhalation. Blood-Composition, grouping and R_h factor-blood pressure. Haemoglobin- functions –anaemia-causes and treatment.

Unit - II: Common Drugs

- 2.1 Antibiotics, Uses and side effects of penicillin, Streptomycin, Chloramphenicol and tetracyclines. Analgesics, Anti-inflammatory drugs and Antipyretics: Paracetamol, Aspirin, Brufen, methyl salicylate
- 2.2 Antiseptics and Disinfectants: Examples and uses. Antihistamines, Hypnotics and Antidepressant drugs-definition, examples and side effects. Anaesthetic-meaning and classification-examples and side effects.

Unit - III: Vital Ailments and Treatment

- 3.1 Epilepsy and Parkinsonism: Causes, Symptoms and treatment. Cancer: Causes, Symptoms and treatment
- 3.2 Tetanus, Tuberculosis, Typhoid and Jaundice: Causes, Symptoms and treatment. Diabetes-meaning, types, causes and symptoms-treatment.AIDS – Causes, Spread and prevention.

Unit - IV: Indian Medicinal Plants & Medicinally Important Compounds 6 Hours

- 4.1 Vallarai, Kizhanelli, Thuslai, Cloves, Ginger, Aloe Vera -medicinal uses.Medicinal benefits of table salt, honey, lemon, coriander, pepper and curry leaves.
- 4.2 Vitamins classification, sources and deficiency diseases of A,D,E and K. Aluminium hydroxide gel, Milk of magnesia, Ferrous gluconate- uses.Biological role of Na, K, Ca, Zn and Cu

Unit - V: First Aid, Safety and Drug Abuse

- 5.1 First aid for shock, haemorrhage, cuts and wounds. Burns-classification and first aid. First aid for fractures, snake bites, poisons, antidotes for poison
- 5.2 Common mental disorders Hysteria, depression. Psychotropic drugs: LSD, Morphineadverse effects.Evil effects of alcohol, tobacco and cannabis.

References

- 1. Jayashree Ghosh, *Textbook of Pharmaceutical chemistry*, Rajendraravindra printers pvt. Ltd., New Delhi, 2010
- 2. James Cross land, Lewis, *Pharmacology*, 5th Edition, Churchill Livingstone Publications, New York.1980
- 3. D. Sriram, P. Yogeeswari, *Medicinal Chemistry*, Second edition, Pearson publications, 2007
- 4. Alex Gringauz, Introduction to Medicinal chemistry, Wiley India Pvt Ltd., New Delhi, 2011.
- 5. Burger, *Medicinal Chemistry and Drug Discovery, Vol-1*, Ed. M. E. Wolff, John Wiley, 1994.
- 6. Goodman & Gilman. Pharmacological Basis of Therapeutics, McGraw-Hill, 2005.
- 7. S. S. Pandeya& J. R. Dimmock, *Introduction to Drug Design*, New Age International, 2000.
- 8. D. Lednicer, Strategies for Organic Drug Synthesis and Design, John Wiley, 1998.
- 9. Graham & Patrick. *Introduction to Medicinal Chemistry*, 3rd edition. OUP, 2005.

NAAC 5th CYCLE

6 Hours

6 Hours

6 Hours

- 10. Rama Rao Nadendla, Principles of Organic Medicinal Chemistry, 2nd Edition, New Age Publications, 2008.
- 11. Ashutosh Kar, *Medicinal Chemistry*, 2nd Edn, New Age Publications, 2000.

Non - Major Elective - II NCH604 Chemistry in Every Day Life Semester - VI 2 Hrs / week (2 Credits)

Objectives

To appreciate the importance of chemistry in day-to-day appliances

To understand the role of chemicals involved in different substances, their uses and precautions to be taken.

Unit - I: Chemistry in Agriculture

- Soil chemistry- types of soil, composition. Properties of soil, preliminary idea about soil 1.1 water, soil temperature, texture, minerals.
- 1.2 Fertilizers-requisites-composition and types and ill effects. Definition and examples of insecticides, fungicides, herbicides, Toxic effects of pesticides. Introduction to organic farming, benefits and challenges.

Unit - II: Chemistry in Housing and Household

- Major classes of household chemicals-cleaners, pesticides, stain removers, fire 2.1 Composition of Portland Cement-Types of concrete. extinguishers.
- 2.2 Paints Composition and types, Varnishes.Composition of soap, shampoos and detergents.Glass - Variety of glasses and their uses.

Unit - III: Chemical Processing and Preservation of Food

- Chemical Food additives for flavour, colour, sweeteners. Food preservation methods 3.1 and chemicals used Beverages- Chemicals in drinks. Bakery Products- Bread, butter and cheese.
- 3.2 Food adulteration-Adulterants in milk, ghee, oil, coffee powder, tea, asafoetida, chilli powder, pulses and turmeric powder-identification

Unit - IV: Plastics and Ceramics

- 4.1 Polythene, Celluloid, PVC, bakelite, polyesters, resins and their applications.Natural Rubber-Synthetic rubbers-Vulcanisation-definition and its applications.
- 4.2 Novel plastics and their applications. Ceramics as insulators, semi-conductors and super conductors. Biomedical Ceramics

Unit-V: Chemistry of cosmetics

- 5.1 Cosmetic formulations- Skin care, Hair care, Deodorants and antiperspirants. Colour cosmetics- Mascara, eye shadow and eye pencil.
- Sun protection, Nail cosmetics, mouth cosmetics. Perfumes and fragrances 5.2

References

- 1. Kirpal Singh, Chemistry in Daily Life, Second Edition, Prentice-Hall of India private Ltd, New Delhi, 2008.
- 2. C. Jain and Monicka Jain, Engineering Chemistry, Dhanpat Raj Publishing Co., (P) Ltd., New Delhi, 2002.
- 3. Jayashree Ghosh, Textbook of Pharmaceutical chemistry, Rajendraravindra printers pvt. Ltd., New Delhi, 2010

6 Hours

6 Hours

NAAC 5th CYCLE

6 Hours

4. Jayashree Ghosh, *Fundamental concepts of Applied Chemistry*, S Chand Publications, New Delhi, 2006