M.Sc. CHEMISTRY

CHOICE BASED CREDIT SYSTEM (CBCS)

Curriculum and Syllabus
Regular (2016 – 2017)

Enable | Enlighten | Enrich

KARPAGAM UNIVERSITY

(Established Under Section 3 of UGC Act, 1956)

DEPARTMENT OF CHEMISTRY
FACULTY OF ARTS, SCIENCE AND HUMANITIES

KARPAGAM UNIVERSITY

(Deemed University Established Under Section 3 of UGC Act, 1956)
Eachanari (Post), Coimbatore – 641 021, Tamil Nadu, India

Preamble

Karpagam University has initiated several measures to bring equity, efficiency and excellence in the Higher Education System of the University. The measures taken to enhance the quality in higher education include innovation and improvements in curriculum, teaching-learning process, and examination and evaluation systems. The grading system is considered to be better than the conventional marks system and is followed. This will facilitate student mobility across institutions within and across countries and also enable potential employers to assess the performance of students.

Choice Based Credit System (CBCS): The CBCS provides an opportunity for the students to choose courses from the prescribed courses comprising core, elective/minor or skill based courses. The courses will be evaluated following the grading system, which is considered to be better than the conventional marks system.

Outline of Choice Based Credit System:

1. Core Course: A course, which should compulsorily be studied by a candidate as a core requirement is termed as a Core course.

2. Elective Course: Generally a course which can be chosen from a pool of courses and which may be very specific or specialized or advanced or supportive to the discipline/ subject of study or which provides an extended scope or which enables an exposure to some other discipline/subject/domain or nurtures the candidate's proficiency/skill is called an Elective Course.

3. Project work/Dissertation is considered as a special course involving application of knowledge in solving / analyzing /exploring a real life situation / difficult problem.

Objectives of the Programme

The student will acquire a foundation of chemistry of sufficient breadth and depth to enable them to understand and critically interpret the primary chemical literature. It provides a broad foundation in chemistry that stresses scientific reasoning and analytical problem solving with a molecular perspective. The student will learn the laboratory skills needed to design, safely conduct and interpret chemical research. The student will learn professionalism, including the ability to work in teams and apply basic ethical principles. The course also prepares the graduates for employment as chemists as well as to pusue research.

Programme Learning Outcomes (PLO)

a. Students will have a firm foundation in the fundamentals and application of current chemical and scientific theories including those in Analytical, Inorganic, Organic and Physical Chemistries.
b. Students will be able to design and carry out scientific experiments as well as accurately record and analyze the results of such experiments.
c. Students will be skilled in problem solving, critical thinking and analytical reasoning as applied to scientific problems.
d. Students will be able to clearly communicate the results of scientific work in oral, written and electronic formats to both scientists and the public at large.
e. Students will be able to explore new areas of research in both chemistry and allied fields of science and technology.
f. Students will appreciate the central role of chemistry in our society and use this as a basis for ethical behavior in issues facing chemists including an understanding of safe handling of chemicals, environmental issues and key issues facing our society in energy, health and medicine.
g. Students will be able to function as a member of an interdisciplinary problem solving team.
h. The graduate has specific skills in planning and conducting advanced chemical experiments and applying structural-chemical characterisation techniques.
i. Are able to use modern instrumentation and classical techniques, to design experiments, and to properly record the results of their experiment.
j. Are able to use modern library searching and retrieval methods to obtain information about a topic, chemical, chemical technique, or an issue relating to chemistry.

Programme Specific outcome (PSO)

k. A graduate with a Master's degree in Chemistry has in-depth and detailed functional knowledge of the fundamental theoretical concepts and experimental methods of chemistry.
l. Students should have an advanced level understanding of the following areas of chemistry - Analytical, Inorganic, Organic, and Physical Chemistry. They should master graduate level understanding of their major area(s) of research.
m. Students should be able to communicate scientific results in writing and in oral presentation.
n. Students should become proficient in their specialized area of chemistry and acquire the basic tools needed to carry out independent chemical research

Programme Educational Objectives

PEO-1

The Masters in Chemistry will extend your depth and breadth of knowledge in all branches of chemistry, suitable for a professional chemist capable of conducting research.

PEO-2

To carryout research in the trust areas of chemistry. Will be able to communicate effectively the scientific information and research results in written and oral formats, to both professional scientists and to the public.

PEO-3

To motivate critical thinking and analytical skills to solve complex chemical problems and the Ability to handle problems of practical relevance to society while complying with economical, environmental, ethical, and safety factors.

PEO-4

To practice chemistry by performance of experiments in the laboratory classes. To perform accurate quantitative measurements with an understanding of the theory and use of contemporary chemical instrumentation, interpret experimental results, perform calculations on these results and draw reasonable, accurate conclusions

Mapping

PO	a	b	c	d	e	f	g	h	i	j	k	l	m	n
PEO 1	x	x			x			x	x		x	x	x	
PEO 2		x	x	x	x			x	x		x		x	x
PEO 3			x	x		x	x			x			x	x
PEO 4	x	x	x			x		x		x	x	x		x

KARPAGAM UNIVERSITY
DEPARTMENT OF CHEMISTRY
M.Sc. CHEMISTRY
(Scheme of Examination for 2016-2017 onwards)

Code	Course(s)	Objectives and outcomes		Ins*	Marks			Exam Hrs	Credit
		PEO'S	PO'S		CIA	ESE	Total		
	SEMESTER – I								
16CHP101	Organic Chemistry – I (Reaction Mechanisms)	1,2,3	a,c,e	4	40	60	100	3	4
16CHP102	Inorganic Chemistry –I (Nuclear Chemistry and Metallic Clusters)	1,2,3	a,c,e	4	40	60	100	3	4
16CHP103	Physical Chemistry- I (Quantum Chemistry and Group Theory)	1,2,3	a,c,e	4	40	60	100	3	4
16CHP104	Organic and Inorganic Spectroscopy	1,2,3,4	a,b,c,h.j	4	40	60	100	3	4
16CHP105A 16CHP105B 16CHP105C	Elective I	1,2,3	a,c,e	4	40	60	100	3	4
16CHP111	Organic Chemistry Practical-I (Qualitative Analysis and Single Stage Preparations)	3,4	b,h,j	4	40	60	100	6	2
16CHP112	Organic Chemistry Practical-II (Quantitative Analysis and Double Stage Preparations)	3,4	b,h,j	4	40	60	100	6	2
	Journal Paper Analysis & Presentation	1,2,3	a,b,c,d,e,h,j	2	-	-	-	-	-
Semester total				**30**	**280**	**420**	**700**		**24**
	SEMESTER – II								
16CHP201	Organic Chemistry-II (Rearrangements, Reactions, Photochemistry and Pericyclic Reactions)	1,2,3	a,c,e	4	40	60	100	3	4
16CHP202	Inorganic Chemistry-II (Co-ordination Chemistry)	1,2,3	a,c,e	4	40	60	100	3	4
16CHP203	Physical Chemistry II (Chemical Kinetics and Electrochemistry)	1,2,3	a,c,e	4	40	60	100	3	4
16CHP204	Industrial chemicals and environment	3,4	f,h	4	40	60	100	3	4
16CHP205A	Elective – 2 (CBCS)	1,2,	a,c,	4	40	60	100	3	4

16CHP205B 16CHP205C		3	e						
16CHP211	Inorganic Chemistry Practical-I (Qualitative Analysis and Preparations)	3,4	b,h, j	4	40	60	100	6	2
16CHP212	Inorganic Chemistry Practical-II (Quantitative Analysis and Complex Preparations)	3,4	b,h, j	4	40	60	100	6	2
	Journal Paper Analysis & Presentation	1,2, 3	A,b, c,d, e,h,j	2	-	-	-	-	-
Semester total					**280**	**420**	**700**		**24**
	SEMESTER – III								
16CHP301	Organic Chemistry-III (Natural Products)	1,2, 3	a,c, e	4	40	60	100	3	4
16CHP302	Physical Chemistry –III (Thermodynamics)	1,2, 3	a,c, e	4	40	60	100	3	4
16CHP303	Physical Methods in Chemistry (Instrumentation)	1,2, 3	a,c, e	4	40	60	100	3	4
16CHP304	Nanochemistry	3,4	F,h	4	40	60	100	3	4
16CHP305A 16CHP305B 16CHP305C	Elective –3 (CBCS)	1,2, 3	a,c, e	4	40	60	100	3	4
16CHP311	Physical Chemistry Practical I (Molecular Weight Determination and Conductometric Titrations)	3,4	b, h,i	4	40	60	100	6	2
16CHP312	Physical Chemistry Practical II (Chemical Kinetics and Potentiometric Titrations)	3,4	b, h,i	4	40	60	100	6	2
	Journal Paper Analysis & Presentation	1,2, 3	A,b, c,d, e,h,j	2	-	-	-	-	-
Semester total				**30**	**280**	**420**	**700**		**24**
	SEMESTER – IV								
	Project and Viva Voce	1,2, 3	A,b, c,d, e,h,j	-	80	120	200	-	15
Semester total				-	80	120	**200**	**-**	**15**
				90	**920**	**1380**	**2300**		**87**

List of Core Course Elective					
Elective-I		**Elective-II**		**Elective-III**	
Code	**Course**	**Code**	**Course**	**Code**	**Course**
16CHP105A	Green Chemistry	16CHP205A	Research methodology for chemistry	16CHP305A	Polymer Chemistry
16CHP105B	Medicinal Chemistry	16CHP205B	Analytical Chemistry	16CHP305B	Textile Chemistry
16CHP105C	Molecular Modelling & Drug Design	16CHP205C	Organometallic Chemistry	16CHP305C	Industrial Chemistry

Semester-I

16CHP101 ORGANIC CHEMISTRY- I 4H 4C
(REACTION MECHANISMS)

Instruction Hours/week: L: 4 T: 0 P: 0 Marks: Internal: 40 External: 60 Total:100

Course Objectives

- To understand aromaticity.
- To provide a versatile knowledge of different name reactions and their application in synthesis.
- To learn about familiar addition and elimination reactions.
- To gain knowledge about reaction intermediates.
- To understand the principles and reaction mechanisms involving various electrophilic and nucleophilic, addition and elimination reactions.
- To relate the different organic reaction mechanisms.

Course outcomes (CO's)

1. Learned the concept aromaticity and various types of aromaticity
2. Familiarized the various types of electrophilic and nucleophilic substitution reactions and their Mechanism
3. Learned the familiar addition and elimination reactions
4. Learned the concept of reaction intermediates.
5. Understood about the synthesise aromatic compounds using electrophilic and nucleophilic substitution, addition and elimination reactions.
6. Described the various organic reaction mechanisms.

Methodology

Blackboard teaching, Powerpoint presentation and group discussion.

UNIT – I

Aromaticity and chemical methods in mechanisms: Aromaticity - introduction - aromaticity of benzenoid and heterocyclic compounds. Non-benzenoid aromatics – annulenes, azulenes, ferrocenes and fulvenes.

Kinetic and non-kinetic methods of study of reaction mechanisms - kinetic methods- Primary and secondary kinetic isotopic effects. Non-kinetic methods - study of intermediates, isotopic labeling, stereochemical studies, energy profile diagrams and cross over experiments. Hammond's postulate. Kinetic and thermodynamic control.

Linear free energy relationship - Hammett equation and Taft equation.

UNIT – II

Addition reactions: Electrophilic, nucleophilic and free radical addition to double and triple bonds - hydration, hydroxylation, Michael addition, hydroboration and epoxidation. Addition reactions to carbonyl compounds – Mannich reaction, Meerwein Pondroff-

Verley reduction, Grignard, Claisen, Dieckmann, Stobbe, Knovenagel, Darzen, Wittig, Thorpe and Benzoin reactions.

UNIT – III

Electrophilic substitution reactions: Aromatic electrophilic substitution reactions-formylations–Gattermann, Gattermann Koch and Riemer Tiemann reactions. Kolbes, Bischler-Napieralski and Hofmann-Martius reactions. Friedel crafts alkylation and acylations and Vilsmeier-Haack reaction.

Aliphatic electrophilic substitution reactions - mechanisms- SE1, SE2 and SEi - structure reactivity relationship, typical electrophilic substitution reactions - Friedel crafts acylation at olefinic carbon, Stork enamine reaction and decarboxylation of aliphatic acids.

UNIT – IV

Nucleophilic substitution reactions: Aliphatic nucleophilic substitution reactions-mechanisms - SN1, SN2, ion pair and SNi- substitution at vinyl carbon. Stereochemistry of nucleophilic substitution reaction - effect of substrate structure - solvent effects - leaving group effect – nucleophilicity, ambident nucleophiles and ambident substrates-neighbouring group participation.

Aromatic nucleophilic substitution reactions - benzyne mechanism, intermediate complex mechanism and SN1 mechanism, structure reactivity relationship.

Ziegler alkylation and Chichibabin reaction.

UNIT – V

Elimination reactions: Mechanisms - E1, E2, Ei and E1cB mechanisms- stereochemistry of eliminations. Hofmann rule-Saytzeff rule-Bredts rule – Substitution versus Elimination. Typical elimination reaction - Chugaev reaction, Hofmann degradation and Cope elimination.

Carbenes and nitrenes - structure, generation and reactions.

SUGGESTED READINGS:

Text Books:

1. Smith, M. B., & March, J. (2007). *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure* (VI Edition). New Jersey: John Wiley & Sons, Inc., Hoboken.
2. Finar, I. L. (2000). *Organic Chemistry Vol. II: Stereochemistry and the Chemistry of Natural Products* (V Edition). New Delhi: Addison Wesley Longman (Singapore) Pvt. Ltd- Indian Branch.
3. Chatwal, G. R. (2011). *Organic Chemistry of Natural Products Vol. II*. New Delhi: Himalaya Publishing House.

Reference Books

1. Sanyal, S. N. (2006). *Reactions, Rearrangements and Reagents* (IV Edition). New Delhi: Bharathi Bhawan (Publishers and Distributors).
2. Tewari, N. (2011). *Advanced Organic Reaction Mechanism* (III Edition). Kolkata: Books and Allied (P) Ltd.
3. Agarwal, O. P. (2004). *Natural Product Chemistry Vol. II*. Meerut: Goel Publishing House.
4. Chatwal, G. R. (2011). *Organic Chemistry of Natural Products. Vol. I*. New Delhi: Himalaya Publishing House.

Semester-I

16CHP102 INORGANIC CHEMISTRY-I 4H 4C

(NUCLEAR CHEMISTRY AND METALLIC CLUSTERS)

Instruction Hours/week: L: 4 T: 0 P: 0 Marks: Internal: 40 External: 60 Total:100

Course Objectives

- To learn the nuclear structure, stable and unstable atomic nuclei, nuclear reactions and different modes of radioactive decay and also methods for measurements of radioactivity.
- To analyses the various defects and its application on inorganic crystals.
- To understand the detection of radioactive rays and to measure the radiation.
- To learn about the fundamentals of metallic clusters.
- To understand the chemistry of boranes and related compounds.
- To apply the knowledge to know about the various forms of inorganic compounds

Course outcomes

1. Described the basic concepts of nuclear chemistry and types of nuclear reactions.
2. Discriminate the various defects and also known about its application on inorganic crystals
3. Understood the Basics of metallic clusters, preparation, properties and applications of metallic clusters
4. Learned the structure and bonding in molecules / ions and predict the structure of molecules / ions.
5. Described the type of defects in metals and about semi conductors
6. Understood the inorganic and organometallic chemistry, catalysis in the molecular level

Methodology

Blackboard teaching, Powerpoint presentation and group discussion.

UNIT – I

Inorganic chains – rings - cages and clusters (definition and structure) - metal clusters - dinuclear clusters - trinuclear clusters - tetranuclear clusters - hexanuclear clusters – organometallic clusters.

Boranes, boron hydrides (structure and properties) – carboranes - metallocarboranes - Wade's theory -closo-nido and arachno structures - borazines, phosphazenes – Sulphur-Nitrogen ring compounds. Isopoly and heteropoly acids of V, Cr, Mo and W.

UNIT – II

Metallic state-free electron, band and zone theories - non stoichiometry - point defects in solids - Schottky and Frenkel defects - linear effects - dislocation - effects due to dislocation - electrical properties of solids - insulators-intrinsic semiconductors - n and p type and super conductors - ceramics elementary treatment.

Organometallic compounds in homogeneous catalytic reactions-coordinative unsaturation – acid-base behavior reaction – migration of atoms or groups from metal to ligand –

insertion reaction – reactions of coordinated ligands – catalytic reactions of alkenes – isomerisation of alkenes – hydrogenation – hydroformylation and hydrosilation of alkenes – alkene polymerization and oligomerisation – fluxional molecules.

UNIT – III

Nuclear Chemistry - the nucleus - subatomic particles and their properties, binding energy. N/P ratios in stable and meta stable nuclei - different type of nuclear forces - liquid model- shell model. Modes of radioactive decay - α, β and γ decay radiation, electron capture, nuclear isomerism and internal conversion.

UNIT – IV

Experimental methods - Cloud chamber, nuclear emulsion, bubble chamber, proportional counters-G.M counter, scintillation counters, semi conductor detector.
Particle accelerators - Cyclotron, synchrotron, betatron and bevatron.

UNIT – V

Nuclear reactions - Bethes's notation, Q-value, columbic barrier, cross section, different types of nuclear reactions - projectiles capture - particle emission, spallation, fission, fusion, theories of fission, use of fission products, nuclear reactors - fissile and fertile isotopes- U^{233},U^{235},Pu^{239},Th^{232},-atomic power projects in India, stellar energy, synthetic elements - application of radio isotopes - Hot atom chemistry**.**

SUGGESTED READINGS:

Text Books:

1. Huheey, J. E., Keitler, E. A., & Keitler, R. L. (2002). *Inorganic Chemistry-Principles of Structure and Reactivity* (IV Edition). Singapore: Pearson Education.
2. Shekar, C. V. (2005). *A Text Book of Nuclear Chemistry* (I Edition). New Delhi: Dominant publishers and Distributors.
3. Arnikar, H. J. (2003). *Essentials of Nuclear Chemistry* (IV Edition). New Delhi: New Age International Publishers Pvt. Ltd.
4. Chakrabarty, D. K. (2005). *Solid State Chemistry* (I Edition). New Delhi: New Age International Publishers.
5. Cotton, F. A., Wilkinson, G., Murillo, C. A., & Bochmann, M. (1999). *Advanced Inorganic Chemistry* (VI Edition). New York: John Wiley & Sons.

Reference Books:

1. Glasstone, S. (1967). *Source Book on Atomic Energy* (III Edition). New Delhi: East West Press.
2. Gurdeep Raj, (2002). *Advanced Inorganic Chemistry Vol. I* (24^{th} Revised Edition). Meerut: Goel Publishing House.
3. Madan, R. D. (2005). *Modern Inorganic Chemistry*. New Delhi: S. Chand & Co.
4. Puri, B. R., & Sharma, L. R. (2002). *Principles of Inorganic Chemistry*. New Delhi: Shoban Lal & Co.
5. Wahid Malik, Madan. R.D., and Tuli, G.D. (2004). Selected topics in Inorgani Chemistry. New Delhi. S. Chand & Co.

Semester-I

16CHP103 PHYSICAL CHEMISTRY- I 4H 4C
(QUANTUM CHEMISTRY AND GROUP THEORY)

Instruction Hours/week:L: 4 T:0 P:0 Marks: Internal:40 External: 60 Total:100

Course Objectives

- To study the fundamentals and applications of classical mechanics and quantum chemistry
- To understand the structure of an atom and different approximation methods
- To learn the concept of Group theory and their applications.
- To discuss the molecular phenomena and its model problems
- To explain the probabilities, amplitudes, averages, expectation values and observables.
- To analyses the concept of group theory to predict the spectroscopic properties of a molecules

Course Outcomes (CO's)

Students have learned and understood

1. The differences between classical and quantum mechanics. The limitations of classical mechanics.
2. the connection of quantum mechanical operators to observables
3. probabilities, amplitudes, averages, expectation values, and observables
4. how molecular phenomena can be related to model problems
5. the fundamentals of group theory
6. the connection between common approximation methods and standard chemical frameworks (Born-Oppenheimer approximation, molecular orbitals, for example)
7. Identified the point groups of molecules and apply the concept of group theory to predict the spectroscopic properties.

Methodology

Blackboard teaching, Powerpoint presentation and group discussion.

UNIT – I

Failure of classical mechanics and the success of quantum theory in explaining black body radiation and photoelectric effect.

The time dependent and time independent Schrodinger equations - Born's interpretation of the wave function. Requirements of the acceptable wave function.

Algebra of operators. Sums and products of operators - commutator - linear operators- eigen functions and eigen values - correspondence between physical quantities in classical mechanics and operators in quantum mechanics - Hamiltonian operator - angular momentum operator. Quantization of angular momentum and its spatial orientation - average values - postulates of quantum mechanics.

UNIT – II

Particle in a one-dimensional box - quantization of energy - normalization of wave function - orthogonality of the particle in a one-dimensional box wave functions. Illustration of the uncertainty principle and correspondence principle with reference to the particle in a one-dimensional box - particle in a three dimensional box - separation of variables.

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

Solving of Schrodinger equation for a rigid rotor. Rigid rotor model of a diatomic molecule.

UNIT – III

Schrodinger equation for the H-atom (or H-like species)- separation of variables - energy levels. Radial distribution functions - orbitals and orbital shapes. Probability density and radial distribution functions.

Need for approximation methods. The perturbation theory- application of perturbation method to systems such as anharmonic oscillator and He-atom.

The variation method - application of variation method to systems such as anharmonic oscillator and He-atom.

UNIT – IV

Symmetry elements and symmetry operations - definition of identical and equivalent elements configurations - effect of performing successive operations commutative and non-commutative - inverse operations.

Groups and their basic properties - definition of a group - basic properties of a group-definition of abelian - cyclic- isomorphic, finite, infinite groups and subgroup. Symmetry classification of molecules into point groups-Schoenflies symbol (only-difference between point group and space group).

Matrices- Definition of matrix, square matrix, diagonal matrix, null matrix, unit matrix, row matrix, column matrix, symmetric matrix, skew symmetric matrix and conjugate matrix. Multiplication, commutative and non commutative-determination of inverse of a matrix, block multiplication of matrices-addition and subtraction of matrices.

Matrix notations for symmetry operations of C_{2v} and C_{3v} groups-construction of character tables for C_{2v} and C_{3v} point groups**.**

UNIT – V

Definition of reducible and irreducible representations - irreducible representations as orthogonal vectors - direct product rule, the great orthogonality theorem and its

consequences - determinations of the characters for irreducible representation of C_{2v} and C_{3v} point groups using the orthogonality theorem.

Group theory and Vibrational spectroscopy - vibrational modes as basis for group representation - symmetry selection rules for IR and Raman spectra, Mutual exclusion principle - classification of vibrational modes.
Group theory and dipole moment.

SUGGESTED READINGS:

Text Books:

1. Prasad, R. K. (2004). *Quantum Chemistry* (II Edition). New Delhi: New Age International Publishers Pvt. Ltd.
2. Cotton, F. A. (2002). *Chemical Applications of Group Theory* (III Edition). Texas: A Wiley Inter Science Publication.
3. Chandra, A. K. (2002). *Quantum Chemistry* (IV Edition). New Delhi: Tata McGraw – Hill Publishing Company Ltd.
4. House, J. E. (2003). *Fundamental of Quantum Chemistry* (II Edition). New Delhi: Academic Press.
5. Levine, I. N. (2004). *Quantum Chemistry* (V Edition). New Delhi: Pearson Education Pvt. Ltd.

Reference Books:

1. Raman, K.V. (2002). *Group Theory and its Applications to Chemistry*. New Delhi: Tata McGraw Publishing Company.
2. Puri, B. R., Sharma, L. R., & Pathania, M. S. (2013). *Principles of Physical Chemistry* (46th Edition). Jalandar: Vishal Publishing Co.
3. Veera Reddy, K. (2009). *Symmetry and Spectroscopy of Molecules*. New Delhi: New Age International Pvt. Ltd.
4. Atkins, P., & De Paula, J. (2014). *Atkins Physical Chemistry* (X Edition). Oxford: Oxford University Press.

Semester-I

16CHP104 ORGANIC AND INORGANIC SPECTROSCOPY 4H 4C

Instruction Hours/week:L: 4 T:0 P:0 Marks: Internal:40 External: 60 Total:100

Course Objective

This course enables the students

- To learn about Electronic spectroscopy.
- To understand about IR spectroscopy.
- To understand the basic concept of NMR spectroscopy
- To apply the different aspects of NMR spectroscopy to predict the structure of compounds.
- To learn about the mass spectroscopy and Mossbauer spectroscopy.
- To learn about the invaluable tools in synthetic chemistry for the confirmation of known molecules and elucidation of shape and structures of unknown compounds of high complexity with a high degree of certainty.

Course outcomes

On completion of this course, students to have

1. Understood the basic concepts of Electronic and IR spectroscopy.
2. Understood the valuable concepts in NMR spectroscopy.
3. Learned the basic knowledge about Mass spectroscopy.
4. Applied the different aspects of NMR spectroscopy to predict the structure of compounds.
5. Analyzed and identified simple organic molecules by using UV, IR, ^{1}H-NMR and ^{13}C-NMR and Mass spectral data.
6. The students learned how to interpret the spectral data and to identify the structure of the molecules

Methodology

Blackboard teaching, Powerpoint presentation and group discussion.

UNIT- I

Ultraviolet and Visible Spectroscopy: Electronic spectra of diatomic molecules - laws of photochemistry - electronic absorption transitions-correlation of electronic structure with molecular structure - simple chromophoric groups - effects of conjugation - Woodward -Fisher rules for α,β unsaturated carbonyl compounds & dienes - aromatic systems with extended conjugation - applications to organic and inorganic compounds - Instrumentation**.**

UNIT-II

Infrared Spectroscopy: The vibrating diatomic molecules-the simple harmonic oscillator and unharmonic oscillator - the diatomic rotor - factors influencing vibrational frequencies - identification of fundamental groups. Fingerprint region-application to organic and inorganic compounds-Instrumentation**.**

UNIT-III

NMR Spectroscopy: Principle of NMR spectroscopy – description of the PMR instrument, factors affecting chemical shifts-chemical shift equivalence and magnetic equivalence - spin-spin coupling - first order and non first order spectra - Hetero nuclear coupling in ^{1}H NMR - deuterium exchange - high field spectra - double resonance-shift reagents-applications to organic and inorganic compounds. FT NMR.

^{13}C NMR spectroscopy-factors affecting the chemical shifts - broad band and off-resonance decoupling - applications in organic chemistry.

UNIT – IV

Mass Spectroscopy: Principles of mass spectrometry – resolution - description of single focusing and double focusing electron impact mass spectrometers - presentation and analysis of spectra - determination of molecular formulae - Nitrogen rule- Stevenson's rule - isotope abundance analysis - meta stable ions and peaks the molecular ion peak - fragmentation processes - Retro Diels - Alder rearrangement - McLaffertty rearrangement - ortho effect - fragmentation associated with functional groups - aldehydes, ketones, carboxylic acids, esters, amides, alcohols, thiols, amine, ethers, sulphides and halides..

UNIT – V

Mossbauer and Problems: Mossbauer spectroscopy – principles - spectrometer - isomer shift - quadrapole interaction - nuclear zeeman splitting – applications.

Problems involving UV, IR, NMR, Mass spectral data (for compounds not more than 10 carbon atoms).

SUGGESTED READINGS:

Text Books:

1. Jag Mohan. (2007). *Organic Spectroscopy: Principles and Applications* (II Edition). New Delhi: Narose Publishing House.
2. Kemp, W. (2004). *Organic Spectroscopy* (III Edition). New York: Palgrave Macmillan.
3. Sharma, Y. R. (2007). Elementary Organic Spectroscopy: Principles and Chemical Applications (V Edition). New Delhi: S. Chand & Company Limited.
4. Silverstein, R. M., Webster, F. X., & Kiemle, D. (2005). *Spectroscopy of Organic Compounds* (VI Edition). New York: John Wiley & Sons.

Reference Books:

1. Levine, I. N. (2004). *Quantum Chemistry* (V Edition). New Delhi: Pearson Education Pvt. Ltd.
2. Prasad, R. K. (2004). *Quantum Chemistry* (II Edition). New Delhi: New Age International Publishers Pvt. Ltd.
3. Drago, R .S. (1965). *Physical Methods in Inorganic Chemistry*. New York: Reinhold Publishing Corporation.

Semester-I

ELECTIVE I

16CHP105-A GREEN CHEMISTRY 4H 4C

Instruction Hours/week: L: 4 T: 0 P: 0 Marks: Internal: 40 External: 60 Total: 100

Course Objectives

This course enables the students

- To introduce the concept of Green chemistry.
- To understand the basics of Medicinal chemistry.
- To introduce the 12 principles of Green chemistry as well as the tools of Gree chemistry.
- To demonstrate how to evaluate a reaction or process and determine "Greener" alternatives.
- To focus on the application of greener routes to improve industrial processes and to produce important products.
- To understand the greener synthetic pathway to produce pharmacological compounds.

Course outcomes

The student understood the following

1. Designed of chemical products and processes that reduce or eliminate the use and generation of hazardous substances.
2. Created awareness for reducing waste, minimizing energy consumption in organic synthesis.
3. Implemented techniques of green synthesis in organic reactions
4. Used the various alternative resources for green technology in organic synthesis.
5. Understood the various greener synthetic pathways and implement it in the production of pharmacological compounds.
6. Applied the concept of microwaves and ionic liquids in various chemical reactions.

Methodology

Blackboard teaching, Powerpoint presentation and group discussion.

UNIT I

Introduction to Green Chemistry and Principles of Green Chemistry:

What is Green Chemistry? Need for Green Chemistry. Goals of Green Chemistry. Limitations/ Obstacles in the pursuit of the goals of Green Chemistry.
Twelve principles of Green Chemistry with their explanations.

UNIT II

Designing a Green Chemical synthesis:

Designing a Green synthesis using these principles: prevention of waste/ byproducts; maximum incorporation of the materials used in the process into the final products, atom economy, calculation of atom economy of the rearrangement, addition, substitution and elimination reactions. Green solvents– supercritical fluids, water as a solvent for organic

reactions, ionicliquids, fluorous biphasic solvent, PEG, solvent less processes, immobilized solvents and how to compare greenness of solvents.

UNIT III

Energy requirements for reactions – alternative sources of energy: use of microwaves and ultrasonic energy.

Microwave assisted reactions in water: Hofmann elimination, methyl benzoate to benzoic acid, oxidation of toluene and alcohols; microwave assisted reactions in organic solvents. Diels-Alder reaction and decarboxylation reaction.
Ultrasound assisted reactions: sonochemical Simmons-Smith Reaction (Ultrasonic alternative to iodine).

UNIT IV

Green synthesis/reaction: Green starting materials, Green reagents, Green solvents, reaction conditions, Green catalysis and Green synthesis- Real world cases (Traditional processes and green ones) Synthesis of Ibuprofen, Adipic acid , disodium iminodiacetate (alternative to Strecker synthesis).

UNIT V

Hazard assessment and mitigation in chemical industry: Future trends in Green Chemistry-oxidation-reduction reagents and catalysts; biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; Noncovalent derivatization. Biomass conversion, emission control and biocatalysis.

SUGGESTED READINGS:

Text Books:

1. Ahluwalia, V. K., & Kidwai, M. (2007). *New Trends in Green Chemistry* (II Edition). New Delhi: Anamalaya Publisher.
2. Anastas, P. T., & Warner, J. C. (1998). *Green Chemistry: Theory and Practice*. Oxford: Oxford University Press.
3. Matlack, A. S. (2001). *Introduction to Green Chemistry*. New York: Marcel Dekker.
4. Cann, M. C., & Connely, M. E. (2000). *Real-World cases in Green Chemistry*. Washington: American Chemical Society.

Reference Books:

1. Ryan, M. A., & Tinnesand, M. (2002). *Introduction to Green Chemistry*, Washington: American Chemical Society.
2. Lancaster, M. (2010). *Green Chemistry: An Introductory Text* (II Edition). Cambridge: RSC Publishing.

3. Clark, J. H, & Macquarrie, D. J. (2002). *Handbook of Green Chemistry & Technology*. Abingdon: Blackwell Publishing.

Semester-I

ELECTIVE I

16CHP105-B MEDICINAL CHEMISTRY 4H 4C

Instruction Hours/week: L: 4 T: 0 P: 0 Marks: Internal: 40 External: 60 Total:100

Course Objectives

This course enables the students

- To understand the basics of Medicinal chemistry.
- To know the drug targets, drug metabolism and about clinical training..
- To understand the in-silico techniques involved in drug development.
- To clear discussion about membrane and receptors in drug delivery process.
- To apply the various theoretical laws to predict the pharmaco-kinetics of the compounds.
- To analyses the molecular receptor binding and molecular recognition of the natural and synthetic compounds.

Course Outcomes

On the completion of the course, students to

1. Understood the basics of Medicinal chemistry.
2. Knew the drug targets, drug metabolism and about clinical training.
3. Understood in-silico techniques involved in drug development.
4. Discussed about membrane and receptors in drug delivery process.
5. Applied the various theoretical laws to predict the pharmaco-kinetics of the compounds.
6. Analyzing the molecular receptor binding and molecular recognition of the natural and synthetic compounds.

Methodology

Blackboard teaching, Powerpoint presentation and group discussion.

UNIT I

Drug discovery, design and development: Synthesis of the representative drugs of the following classes: analgesic, antipyretic and anti-inflammatory agents (Aspirin, paracetamol and lbuprofen); antibiotics (Chloramphenicol); antibacterial agents (Sulphonamides), antiviral agents (Acyclovir), Central Nervous System agents (Phenobarbital and Diazepam).

UNIT II

Insilco Drug Design and Computer Assisted New Lead Design: Introduction, historical perspective, drug compounds, preparation and organization for drug seeking, common stages in the drug seeking campaign, sources of hits, leads and candidate drugs, natural products: higher plant and animal products, combinational libraries, lead optimization. Introduction, basic concepts, molecular recognition by receptor and ligand design, active conformation, approaches to discover new functions, approaches to the cases with known and unknown receptor structure and molecular docking study.

Introduction to drug metabolism, toxicity and pharmacokinetics, toxicology considerations, problems and drawbacks on drug discovery and development.

UNIT III

Membranes and Receptors: Drug transport mechanism and absorption processes, pharmacodynamic and pharmacokinetic aspects, prodrugs and bioactivation, receptor theories and receptor models, drug receptor interactions drug design, physiochemical principles and basis of drug design, different methods of drug design,

UNIT IV

QSAR: Electronic effects; Hammett equation, Lipophilicity effects; Hansch equation, Steric Effects; Taft Equation; Experimental and theoretical approaches for the determination of physico-chemical parameters, parameter inter-dependence; linearity versus non-linearity; The importance of biological data in the correct form; Molecular docking and dynamics: Rigid docking, flexible docking and manual docking.

UNIT V

Molecular Recognition in Drug-Receptor Binding: Molecular forces and binding energetic, enzyme inhibitors - modes of inhibition and general approaches. Antibacterial drugs - major drug classes and drug resistance, antiviral drugs- major drug classes and drug resistance, anticancer drugs- major cancer drug targets, major drug classes and drug resistance.

SUGGESTED READINGS:

Text Books:

1. Ahluwalia, V. K. (2012). *Green Chemistry-Environmentally Benign Reactions*. New Delhi: Ane Books Pvt Ltd.
2. Ghose, J. (2005). *A Text book of Pharmaceutical Chemistry*. New Delhi: S. Chand Pub Ltd.
3. Ilango, K., & Valentina, P. (2007). *Text Book of Medicinal Chemistry. Vol I*. Chennai: Keerthi Publishers.
4. Ashutosh Kar, (2005). *Medicinal Chemistry* (III Edition). New Delhi: New Age International Publishers.

Reference Books:

1. Stanley E. Manahan, (2006). *Green Chemistry and the Ten Commandments of Sustainability* (II Edition). Columbia, Missouri U.S.A: ChemChar Research. Inc Publishers Columbia.
2. Chatterjea, M. N., & Shinde, R. (2012). *Textbook of Medicinal Biochemistry*. New Delhi: Jaypee Brothers. Medical Publishers (P) Ltd**.**
3. G.L. Patrick, (1995). *Introduction to Medicinal Chemistry* (I Edition). UK: Oxford University Press.
4. Wermuth, C. G. (1992). *Medicinal Chemistry for the 21st Century*. Oxford: Blackwell.

Semester-I

ELECTIVE I

16CHP105-C MOLECULAR MODELLING & DRUG DESIGN 4H 4C

Instruction Hours/week: L:4 T:0 P:0 Marks: Internal:40 External: 60 Total:100

Course Objectives

This course enables the students

- To the students should be acquainted with theoretical and practical knowledge of molecular modeling tools and techniques for drug design and discovery.
- To get knowledge of molecular modeling software will be useful for commercial projects related to drug discovery and developments.
- To understand the detailed knowledge and skill is given in the course and the students get acquired the same after studying the course.
- To study about the importance of pharmacophores in drug discovery process.
- To practice some online softwares to predict the physical and biological properties of natural/synthesized molecules.
- To apply the in-silico techniques to evaluate the drug-receptor binding affinities of the compounds.

Course outcomes (CO's)

On completion of this course, students have

1. Gained the knowledge on the molecular modeling and field effects as a part of drug discovery.
2. Understood on the various stages and various targets of drug discovery.
3. Learned the importance of the pharmacophores in drug discovery.
4. Studied the importance of the role of computer aided drug design in drug discovery.
5. Practiced some online softwares to predict the physical and biological properties of natural/synthesized molecules.
6. Applied the in-silico techniques to evaluate the drug-receptor binding affinities of the compounds.

Methodology

Blackboard teaching, Powerpoint presentation and group discussion.

UNIT I

Introduction to Molecular Modelling:

Introduction-Useful concepts in molecular modelling: Coordinate systems.
Potential energy surfaces. Molecular graphics. Surfaces. Computer hardware and software. The molecular modelling literature.

UNIT II

Force Fields:

Fields. Bond stretching. Angle bending. Introduction to nonbonded interactions.
Electrostatic interactions. Van der Waals Interactions. Hydrogen bonding in molecular mechanics. Force field models for the simulation of liquid water.

UNIT III

Basics of molecular modelling, methods, steps involved in MM, selection of target and template, homology modelling, refinement and validation-SAVES server, the critical assessment of protein structure prediction (CASP), superposition of proteins using different tools, RMSD, presentation of protein conformations, hydrophobicity factor, shape complementary.

UNIT IV

Pharmacophore

Historical perspective and viewpoint of pharmacophore, functional groups considered as pharmacophores, Ehrlich's "Magic Bullet", Fischer's "Lock and Key", two-dimensional pharmacophores, three-dimensional approach of pharmacophores, criteria for pharmacophore model, pharmacophore model generation software tools, molecular alignments, handling flexibility, alignment techniques, scoring and optimization, pharmacophores, validation and usage, automated pharmacophore generation methods, GRID-based pharmacophore models, pharmacophores for hit identification, pharmacophores for human ADME/tox-related proteins.

UNIT V

Computer aided Chemistry: Structure Prediction and Drug Design:

Introduction to molecular docking, rigid docking, Flexible docking, manual docking, advantage and disadvantage of flex-X, flex-S, AUTODOCK and other docking software, scoring functions, simple interaction energies, GB/SA scoring (implicit solvation), CScore (consensus scoring algorithms).

SUGGESTED READINGS:

Text Books:

1. Leach, A. R. (2001). *Molecular Modelling Principles and Application* (II Edition). Longman: Prentice Hall.
2. Haile, J. M. (1997). *Molecular Dynamics Simulation Elementary Methods* (I Edition). UK: John Wiley and Sons.

Reference Books:

1. Gupta, S. P. (2008). *QSAR and Molecular Modeling* (I Edition). Springer-Netherlands: Anamaya Publishers.

Semester -I

16CHP111 ORGANIC CHEMISTRY PRACTICAL-I 4H 2C
(QUALITATIVE ANALYSIS AND SINGLE STAGE PREPARATIONS)

Instruction Hours/week:L: 0 T:0 P:4 Marks: Internal:40 External: 60 Total:100

Course Objectives

The course enables the students should have

- To learn about the qualitative analysis by semi micro-qualitative analysis method.
- To learn the preparation of inorganic complexes.
- To describe the basic concept and advantages of semi- micro qualitative analysis.
- To understand the systematic separation d-block elements
- To study the step wise procedure to predict the anions along with metals
- To identify the d-block elements with their special tests.

Course Outcomes

Students have to,

1. Learned about the qualitative analysis by semi micro-qualitative analysis method.
2. Learned the preparation of inorganic complexes.
3. Described the basic concept and advantages of semi- micro qualitative analysis.
4. Understood the systematic separation d-block elements
5. Studied the step wise procedure to predict the anions along with metals
6. Identified the d-block elements with their special tests.

Methodology

Blackboard teaching and Demonstration.

Contents

Analysis of two – component mixtures: Separation and characterization of compounds.

Note: Each student should analyze a minimum of six organic mixtures.

Preparations involving one stage comprising of the following process: Nitration, acylation, halogenation, diazotisation, rearrangement, hydrolysis, reduction, alkylation and oxidation and one preparation illustrating the following: Benzoin condensation, Canizzaro reaction, Perkin reaction, Reimer-Tiemann reaction, Sandmayer reaction, Fries rearrangement, Skraup synthesis- single stage.

Note: Each student should do a minimum of six preparations involving single stage.

SUGGESTED READINGS:

Text Books:

1. Thomas, A. O., (2003). *Practical Chemistry*. Cannanore: Scientific Book Center.
2. Bansal, R. K, (2008). *Laboratory Manual of Organic Chemistry* (IV Edition). New Delhi: New Age Publishers.
3. Arun Sethi, (2003). *Laboratory experiments in Organic Chemistry*. New Delhi: New Age Publisher.

Reference Books:

1. Furniss, B. S., Hannaford, A. J., Smith, P. W. G., & Tatchell, A. R., (2004). *Vogel's Textbook of Practical Organic Chemistry* (V Edition). Singapore: Pearson Education Ltd.
2. Lepse, P. A., & Lyle B. P., (1986). Lab Manual for Lingren's Essentials of Chemistry. New Delhi: Prentice Hall.

Semester - I

16CHP112 ORGANIC CHEMISTRY PRACTICAL-II 4H 2C
(QUANTITATIVE ANALYSIS AND DOUBLE STAGE PREPARATIONS)

Instruction Hours/week:L: 0 T:0 P:4 Marks: Internal:40 External: 60 Total:100

Course Objectives

Course enables the students should have

- To learn about the basic principles about quantitative analyses.
- To study the concepts and systematic procedure in gravimetric analysis.
- To must know about the systematic procedure for estimation.
- To describe the synthesis method for in-organic co-ordination complexes
- To separate the molecules and identify its nature through chromatography technique.
- To apply this ideas and concepts to water treatment process, food science and forensic fields.

Course Outcomes

On successful completion of the course the students should have

1. Learned about the basic principles about quantitative analyses.
2. Studied the concepts and systematic procedure in gravimetric analysis.
3. Knew about the systematic procedure for estimation.
4. Described the synthesis method for in-organic co-ordination complexes
5. Known about separate the molecules and identify its nature through chromatography technique.
6. Applied this ideas and concepts to water treatment process, food science and forensic fields.

Methodology

Blackboard teaching and Demonstration.

Contents

Estimation of phenol, ethyl methyl ketone, glucose, nitro, amino and methoxy groups, unsaturation in an organic compound.

Analysis of oils Reichert- Meissl value, Iodine value, saponification value and acetyl value.

Double stage preparations- Anthranilic acid and pthalimides.

Extraction and estimation of active constituents

Only for learning purpose and demo (Not for exam)

a. Lactose from milk.
b. Caffeine from tea.
c. Nicotine from tobacco extract.
d. Citric acid or ascorbic acid from a tablet or from a natural source.
e. Curcumin from turmeric.
f. Lycopene from tomato.

SUGGESTED READINGS:

Text Books:

1. Arun Sethi, (2003). *Laboratory experiments in Organic Chemistry*. New Delhi: New Age Publisher.
2. Bansal, R. K, (2008). *Laboratory Manual of Organic Chemistry* (IV Edition). New Delhi: New Age Publishers.
1. Furniss, B. S., Hannaford, A. J., Smith, P. W. G., & Tatchell, A. R., (2004). *Vogel's Textbook of Practical Organic Chemistry* (V Edition). Singapore: Pearson Education Ltd.

Reference Books:

1. Lepse, P. A., & Lyle B. P., (1986). *Lab Manual for Lingren's Essentials of Chemistry*. New Delhi: Prentice Hall.
2. Mendham, J., Denney, R. C., Barnes, J.D., & Thomas, M. (2002). *Vogel's textbook of quantitative Chemical Analysis* (VI Edition). Singapore: Pearson Education Ltd.

Semester - II

16CHP201 ORGANIC CHEMISTRY-II 4H 4C

(REARRANGEMENTS, REACTIONS, PHOTOCHEMISTRY AND PERICYCLIC REACTIONS)

Instruction Hours/week:L: 4 T:0 P:0 Marks: Internal:40 External: 60 Total:100

Course Objectives

This course enables the students

- To know about versatile knowledge of rearrangements
- To understand the different organic (radical and concerted) reactions and their applications in synthesis.
- To learn the principles of conformational analysis and stereochemistry.
- To explain the concepts in organic photochemistry
- To describe the basic ideas about pericyclic reactions
- To implement this basic concept to design and produce the new organic molecules

Course outcomes (CO's)

On successful completion of the course the students should have

1. Understood the versatile knowledge of rearrangements
2. Understood the different organic reactions (radical and concerted).
3. Learned about the principle of conformational analysis and stereochemistry.
4. Explained about the molecular rearrangements, Pericyclic reactions and Cyclo addition and sigmatropic reactions
5. Described the basic ideas of pericyclic reactions.
6. Designed new form of organic compounds using these basic concepts.

Methodology

Blackboard teaching, Powerpoint presentation and group discussion.

UNIT – I

Molecular rearrangements: Intramolecular 1,2 - shifts - Wagner - Meerwein and Pinacol-Pinacolone rearrangements.

Migration to carbonyl carbon – Demyanov and Neber rearrangements.

Rearrangements to electron deficient nitrogen and oxygen – Baeyer – Villiger, Dienone - phenol, Favorskii, Fries, Wolff, Benzidine, Hoffmann Rearrangement and Stevens rearrangements.

Non-cyclic rearrangements – Chapman and Wallach rearrangements**.**

UNIT – II

Conformational analysis and stereochemistry: Stereochemistry of sulphur and nitrogen compounds, stereoselective and stereospecific reactions - R/S-notation of optically active carbon compounds. Optical isomerism of biphenyls, allenes and spiranes. Planar chirality - cyclophanes and ansa compounds - geometrical isomerism - E/Z notation-configuration in aldoximes and ketoximes. Conformation in cyclic system– decalins, perhydrophenanthrene and perhydroanthracene. Conformation and reactivity of cyclohexanes.

UNIT – III

Radical reactions: Configuration and generation of short lived free radicals- characteristics of free radical reactions – radical substitution, radical additions and rearrangement of free radicals. Typical reactions such as Sandmeyer, Gomberg, Pechmann, Ullmann, Pschorr and Hunsdiecker reactions.

Oxidation and reductions- mechanisms – aromatisation, oxidation of alcohols and glycols, ozonolysis, Sommelet reaction and selectivity in reduction-metal hydride reduction- reduction of nitro compounds and acyloin condensation.

UNIT – IV

Organic photochemistry: Introductory theory of light absorption- Jablonski diagram- photophysical processes- excimers and exciplexes - energy transfer-geometry of excited states – quantum efficiency - photochemical reaction of ketones- Norrish type-I and type-II reactions. Paterno Buchi reaction- cis and trans isomerisation-Photo-Fries rearrangement and Ene reaction and Di-pi methine rearrangement.

UNIT – V

Pericyclic reactions: Definition-classification-characteristic features- the electrocyclic reaction-Woodward – Hofmann rules- orbital correlation diagram- the Frontier molecular orbital theory-electrocyclic conversion of 1,3-dienes and 1,3,5-trienes. Cycloaddition – [2+2] addition-Diel's Alder reaction- stereochemistry of Diel's Alder reaction. Sigmatropic reactions – [1,3], [1,5] and [3,3] sigmatropic shifts - Cope and Claisen rearrangements.

SUGGESTED READINGS:

Text Books:

1. Smith, M. B., & March, J. (2007). *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure* (VI Edition). New Jersey: John Wiley & Sons, Inc., Hoboken.
2. Mukherji, S. M., & Singh, S. P. (2002). *Reaction Mechanism in Organic Chemistry* (III Edition). New Delhi: Rajiv Beri for Macmillan India Ltd.
3. Nasipuri, D. (2003). *Stereochemistry of Organic Compounds: Principles and Applications* (II Edition). New Delhi: New Age International (P) Ltd.
4. Tewari, N. (2011). *Advanced Organic Reaction Mechanism* (III Edition). Kolkata: Books and Allied (P) Ltd.

Reference Books:

1. Sanyal, S. N. (2006). *Reactions, Rearrangements and Reagents* (IV Edition). New Delhi: Bharathi Bhawan (Publishers and Distributors).
2. Ramesh, P. (2005). *Basic Principles of Organic Stereochemistry* (I Edition). Madurai: Meenu Publications.
3. Depuy, C. H., & Chapman, O. L. (1975). *Molecular Reactions and Photochemistry* (II Edition). New Delhi: Prentice-Hall of India Private Limited.

4. Coxon, J. M., & Halton, B. (1987). Organic Photochemistry (II Edition). London: Cambridge University Press.
5. Nicholass, J. T., Scaiano J. C., & Ramamurthy, V. (2010). *Modern Molecular Photochemistry of Organic Molecules* (I Edition). United States: University Science Books.

Semester-II

16CHP202 INORGANIC CHEMISTRY- II 4H 4C
(CO-ORDINATION CHEMISTRY)

Instruction Hours/week:L: 4 T:0 P:0 Marks: Internal:40 External: 60 Total:100

Course objectives

This course enables the students

- To understand the theories of bonding in coordination compounds.
- To study the kinetics and mechanisms of reactions of complex compounds.
- To understand the magnetic properties of coordination compounds.
- To learn about the coordination compounds present in the biological systems and their functions.
- To remember the types of coordination compounds like metal carbonyls, carbocyclic pi complex in coordination compounds
- To evaluate the geometries of simple molecules.

Course Outcomes

On the completion of this course, students should have to

1. Learned how to name coordination compounds and to be able to draw the structure based on its name
2. Used Crystal Field Theory to understand the magnetic properties (and in simple terms the colour) of coordination compounds
3. Described the stability of metal complexes by the use of formation constants and to calculate thermodynamic parameters from them
4. Recognized the types of coordination compounds like metal carbonyls, carbocyclic pi complexes in coordination compounds
5. Familiar with some reactions and applications of coordination compounds
6. Predicted the geometries of simple molecules

Methodology

Blackboard teaching, Powerpoint presentation and group discussion.

UNIT-I

Coordination Chemistry: Nomenclature, isomerism and methods of preparation of coordination complexes- types of ligands.

Bonding: Valence bond theory- Crystal field theory – Crystal field effects in tetrahedral, octahedral and square planar symmetries. Crystal field stabilization energy - weak and strong fields- spectrochemical series. Molecular orbital theory: based on group theoretical approach. M.O. diagram of Oh. Td & square planar symmetries involving pi bonding- experimental evidence for the presence of pi bonding. Magnetic behaviour of the transition metal ions in crystal field and molecular orbital theories.

UNIT-II

Electronic spectra of complexes: Term symbols for d configuration. Characteristics of d-d transition and selection rules. Weak and strong field limits. Orgel and Tanabe -

Sugano diagrams. Jahn-Teller tetrahedral distortion and spin orbit couplings. Nephelauxetic effect - charge transfer spectra.

UNIT-III

Metal carbonyls: Methods of preparation, structure, bonding and reactions. Carbonylate ions. Carbonyl hydrides–Vaska's compound, complexes of molecular nitrogen and oxygen. Nitrosyl complexes, dinitrogen complexes. Complexes of unsaturated hydrocarbons- alkenes, allyl and pentadienyl complexes.

UNIT-IV

Carbocyclic pi complexes: Cyclopendienyl and related complexes synthesis, bonding, structure and reaction. Arene complexes-complexes of biochemical importance: Cytochromes, Haemoglobin, Myoglobin, Cyanocobalamine, Chlorophyll- structure and functions.

UNIT-V

Reaction of coordination compounds: Substitution reactions in square planar and octahedral complexes – Trans effect – mechanism of redox reactions.

Homogeneous catalysis by coordination compounds – hydroformylation –carboxylation of methanol – hydrogenation of unsaturated organic compounds.

SUGGESTED READINGS:

Text Books:

1. Huheey, J. E., Keitler, E. A., & Keitler, R. L. (2002). *Inorganic Chemistry-Principles of Structure and Reactivity* (IV Edition). Singapore: Pearson Education.
2. Madan, R. L., & Tuli, G. D. (2005). *Inorganic Chemistry Questions & Answers*. New Delhi: S. Chand and Co.
3. Sarn, K. (2005).*Co-ordination Chemistry*. New Delhi: Rajat Publications.
4. Catherine, E. H., & Alan G. S. (2012). *Inorganic Chemistry* (IV Edition). England: Pearson Education Limited, Harlow.
5. Cotton, F. A., Wilkinson, G., & Paul. L. (2002). Basic Inorganic Chemistry (III Edition). New York: John Wiley & Sons.

Reference Books:

1. Agarwal, R. C. (1998). *Some Recent Aspects of Inorganic Chemistry*. Allahabad: Kitab Mahal.
2. Chakraburty, D. K. (2003). *Inorganic Chemistry*. New Delhi: New Age International Publishing Pvt. Ltd.
3. Cotton, F. A., Wilkinson, G., Murillo, C. A., & Bochmann, M. (1999). *Advanced Inorganic Chemistry* (VI Edition). New York: John Wiley & Sons.
4. Drago, R. S. (1965). *Physical Methods in Inorganic Chemistry*. New York: Rein Gold Publishing Corporation.

Semester-II

16CHP203 PHYSICAL CHEMISTRY- II 4H 4C

(CHEMICAL KINETICS AND ELECTROCHEMISTRY)

Instruction Hours/week:L: 4 T:0 P:0 Marks: Internal:40 External: 60 Total:100

Course Objectives

This course enables the students

- To provide knowledge on fundamental understanding of chemical kinetics and to establish a relationship between the rate of reaction and the concentration of the reactants (the rate law, or rate equation).
- To apply the chemical kinetics concept to study the enzyme mechanisms.
- To provide knowledge to the students about coulometric methods and its application.
- To investigate the adsorption, classification of adsorption and factors affecting of adsorption over corrosion application.
- To remember the basic polarography concepts.
- To understand the theories of catalysis and types of catalysis.

Course outcomes

On the completion of this course, student have to

1. Student understood theories of reaction rates, how reaction rates are measured and represented in rate laws.
2. Understood the applications of chemical kinetics in studying enzyme mechanisms
3. Provided the knowledge of coulometric methods and applications.
4. Evaluated the electrochemical principles involved in corrosion and energy storage.
5. Remembered the basic polarography techniques.
6. Understood the theories of catalysis and types of catalysis

Methodology

Blackboard teaching, Powerpoint presentation and group discussion.

UNIT-I

Theories of reaction rates: Arrhenius theory- hard - sphere collision theory of gas – phase reactions. Activated complex theory or Absolute reaction rate theory (ARRT) for ideal gas reactions (in terms of partition functions).

Reactions in solution: Comparison between gas-phase and solution reactions. The influence of the solvent on the reactions between ions. Influence of ionic strength on rates of reactions in solution - primary salt effect-influence of pressure on rates of reactions in solution -significance of volume and entropy of activations.

Study of fast reactions: Flow methods, pulse methods, relaxation methods, shock-tube method and nuclear magnetic resonance method.

UNIT-II

Homogeneous catalysis: Specific and general acid - base catalysis. Bronsted catalysis law- Hammett acidity functions. Enzyme catalysis (single substrate reaction only). Michaelis Menten law - Influence of pH and temperature on enzyme catalysis.
Surface phenomenon and heterogeneous catalysis: Adsorption and free energy relation at interfaces. Gibb's adsorption isotherm- physisorption and chemisorptions- Adsorption isotherms (Freundlich & Langmuir). Kinetics of heterogeneous catalysis- Langmuir - Hinshelwood and Langmuir - Rideal - Eley mechanisms.

UNIT-III

Inter ionic attraction theory: Debye – Huckel – Onsager equation - Falkenhagen effect- Wien effect. Activity and activity coefficient- ionic strength- Debye – Huckel limiting law and its applications.
Theories of double layer. Helmholtz – Perrin - Gouy chapmann – Stern theories**.**

UNIT – IV

Polarography: Current – voltage relationships-the dropping mercury electrode. Diffusion current- half – wave potentials. Applications of polarography- Amperometric titrations.
Fundamental principles of coulometric methods- constant current and controlled potential methods- simple applications.

UNIT – V

Kinetics of corrosion: Importance–graphical presentation of kinetic data-exchange current density- different types of polarization of electrodes. Activation polarization and Tafel plots-mixed potential theory-application of electrode kinetics to experimental observations-faradic impedance and corrosion.

SUGGESTED READINGS:

Text Books:

1. Bahl, A., Bahl, B. S., & Tuli, G. D, (2014). *Essentials of Physical Chemistry* (V Edition). New Delhi: S. Chand & Company.
2. Puri, B. R., Sharma, L.R., & Pathania, M .S. (2015). Elements of Physical Chemistry. Jalandhar: Vishal Publishing House.
3. Laidler, K. J. (2004). *Chemical Kinetics* (III Edition). New Delhi: Pearson Education Publishing. Indian branch.
4. Atkins, P., & De Paula, J. (2014). *Atkins Physical Chemistry* (X Edition). Oxford: Oxford University Press.
5. Glasstone, S. (2002). *An Introduction to Electrochemistry*. New Delhi: Litton Educational Publishing.

Reference Books:

1. Arora, M. G. (1996). *Polarographic Methods in Analytical Chemistry* (I Edition). New Delhi: Anmol Publications.
2. Raj Narayan, (1983). *An Introduction to Metallic Corrosion and Its Prevention* (I Edition). New Delhi: Oxford & IBH Publishing Company.

3. Moore, W. J. (1999). Physical Chemistry (V Edition). Orient Longman Ltd. Prentice Hall-Inc Delhi.
4. Rajaram, J., & Kuriakose, K. C. (1993). *Kinetics and Mechanisms of Chemical Transformations*. Chennai: MacMillan.

16CHP204 INDUSTRIAL CHEMICALS AND ENVIRONMENT 4H 4C

Instruction Hours/week:L: 4 T:0 P:0 Marks: Internal:40 External: 60 Total:100

Course Objectives

The course enables the students to

- Understand the industrial gases and inorganic chemicals which have an impact on the environment.
- Study about the general principles of metallurgy.
- Learn the environment and its segments.
- Discuss about the water pollution and water treatment.
- Explain the application of bio-catalysis in energy saving techniques.
- Apply this technique to design energy saving devices with eco-friendly method.

Course Outcomes

The course enables the students to

1. Understood the industrial gases and inorganic chemicals which have an impact on the environment.
2. Studied about the general principles of metallurgy.
3. Learned the environment and its segments.
4. Discussed about the water pollution and water treatment.
5. Explained the application of bio-catalysis in energy saving techniques.
6. Appling this technique to design energy saving devices with eco-friendly method.

Methodology

Blackboard teaching, Power point presentation and group discussion.

UNIT I

Industrial Gases and Inorganic Chemicals:

Industrial Gases: Large scale production, uses, storage and hazards in handling of the following gases: oxygen, nitrogen, argon, neon, helium, hydrogen, acetylene, carbon monoxide, chlorine, fluorine, sulphur dioxide and phosgene.

Inorganic Chemicals: Manufacture, application, analysis and hazards in handling the following chemicals: hydrochloric acid, nitric acid, sulphuric acid, caustic soda, common salt, borax, bleaching powder, sodium thiosulphate, hydrogen peroxide, potash alum, chrome alum, potassium dichromate and potassium permanganate.

UNIT II

Industrial Metallurgy:

General Principles of Metallurgy:

Chief modes of occurrence of metals based on standard electrode potentials. Ellingham diagrams for reduction of metal oxides using carbon as reducing agent.

Hydrometallurgy, methods of purification of metals (Al, Pb, Ti, Fe, Cu, Ni, Zn): electrolytic, oxidative refining, Kroll process, Parting process, Van Arkel-de Boer

process and Mond's process. Preparation of metals (ferrous and nonferrous) and ultrapure metals for semiconductor technology.

UNIT III

Environment and its segments:

Ecosystems. Biogeochemical cycles of carbon, nitrogen and sulphur.

Air Pollution: Major regions of atmosphere. Chemical and photochemical reactions in atmosphere. Air pollutants: types, sources, particle size and chemical nature; Photochemical smog: its constituents and photochemistry. Environmental effects of ozone, Major sources of air pollution.

Pollution by SO_2, CO_2, CO, NOx, H_2S and other foul smelling gases. Methods of estimation of CO, NO_x, SO_x and control procedures. Effects of air pollution on living organisms and vegetation. Greenhouse effect and Global warming, Ozone depletion by oxides of nitrogen, chlorofluorocarbons and halogens, removal of sulphur from coal. Control of particulates.

Unit IV

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.

Water purification methods. Effluent treatment plants (primary, secondary and tertiary treatment). Industrial effluents from the following industries and their treatment: electroplating, textile, tannery, dairy, petroleum and petrochemicals, agro, fertilizer, etc. Sludge disposal.

Industrial waste management, incineration of waste. Water treatment and purification (reverse osmosis, electro dialysis, ion exchange). Water quality parameters for waste water, industrial water and domestic water.

Unit V

Energy & Environment:

Sources of energy: Coal, petrol and natural gas. Nuclear fusion / fission, solar energy, hydrogen, geothermal, tidal and hydel, etc. Nuclear pollution: Disposal of nuclear waste, nuclear disaster and its management.

Biocatalysis:

Introduction to biocatalysis: Importance in "Green chemistry" and chemical industry.

SUGGESTED READINGS:

Text Books:

1. Stocchi, E. (1990). *Industrial Chemistry Vol-I*. UK: Ellis Horwood Ltd.
2. Felder, R. M., & Rousseau, R. W. (2010). *Elementary Principles of Chemical Processes*. (III Edition). New Delhi. Wiley India Pvt. Ltd
3. Kent, K. A. (1997). Riegel's Handbook of Industrial Chemistry (IX Edition). New Delhi: CBS Publishers and Distributors Private Limited.

Reference Books:

1. Umare, S. S. & Dara, S.S. (2014). *A Textbook of Engineering Chemistry* (V Edition). New Delhi: S. Chand & Company Ltd.
2. De, A. K. (2005). *Environmental Chemistry* (III Edition). New Delhi: New Age International Publishers (P) Ltd.
3. Khopkar, S. M. (1993). *Environmental Pollution Analysis*. New Delhi: Wiley Eastern Ltd.

ELECTIVE-II **Semester - II**

16CHP205A **RESEARCH METHODOLOGY FOR CHEMISTRY** **4H 4C**

Instruction Hours/week:L: 4 T:0 P:0 **Marks: Internal:40 External: 60 Total:100**

Course Objectives

The course enables the students to

- Understand how to do literature survey about a particular scientific problem.
- Learn about the digital sources available for the literature collection.
- Study the methods of doing scientific research and how to write scientific papers.
- Discuss about the chemical safety and ethical handling of chemicals.
- Understand about the data analysis.
- Know about, how to handle the chemicals in safer way and how to analysis the data.

Course Outcomes

On the completion of this course, students to

1. Understood how to do literature survey about a particular scientific problem.
2. Learned about the digital sources available for the literature collection.
3. Studied the methods of doing scientific research and how to write scientific papers.
4. Discussed about the chemical safety and ethical handling of chemicals.
5. Understood about the data analysis.
6. Knew about, how to handle the chemicals in safer way and how to analysis the data.

Methodology

Blackboard teaching, Power point presentation and group discussion.

Unit I

Literature Survey:

Print: Sources of information: Primary, secondary, tertiary sources; Journals: Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text-books, current contents, introduction to chemical abstracts and beilstein, subject index, substance index, author index, formula index, and other indices with examples.

Unit II

Digital: Web resources, E-journals, journal access, TOC alerts, hot articles, citation index, impact factor, H-index, E-consortium, UGC infonet, E-books, internet discussion groups and communities, blogs, preprint servers, search engines, scirus, Google scholar, chemindustry, Wiki-databases, chemspider, science direct, scifinder, Scopus.

Information Technology and Library Resources: The Internet and World Wide Web. Internet resources for chemistry. Finding and citing published information.

Unit III

Methods of Scientific Research and Writing Scientific Papers:

Reporting practical and project work. Writing literature surveys and reviews. Organizing a poster display. Giving an oral presentation.

Writing scientific papers – justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work. Writing ethics. Avoiding plagiarism.

Unit IV

Chemical Safety and Ethical Handling of Chemicals:

Safe working procedure and protective environment, protective apparel, emergency procedure and first aid, laboratory ventilation. Safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmospheric – safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives, identification, verification and segregation of laboratory waste, disposal of chemicals in the sanitary sewer system, incineration and transportation of hazardous chemicals.

Unit V

Data Analysis:

The Investigative Approach: Making and Recording Measurements. SI Units and their use. Scientific method and design of experiments.

Analysis and Presentation of Data: Descriptive statistics. Choosing and using statistical tests.

Chemometrics. Analysis of variance (ANOVA), Correlation and regression, Curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, General polynomial fitting, linearizing transformations, exponential function fit, *r* and its abuse. Basic aspects of multiple linear regression analysis.

Electronics:

Basic fundamentals of electronic circuits and their components used in circuits of common instruments like spectrophotometers, typical circuits involving operational amplifiers for electrochemical instruments. Elementary aspects of digital electronics.

SUGGESTED READINGS:

Text Books:

1. Dean, J., Jones, A. M., Holmes, D., Reed, R., Jones, A., & Weyers, J. (2011). *Practical Skills in Chemistry* (II Edition). Harlow: Prentice-Hall.
2. Hibbert, D. B., & Gooding, J. J. (2006) *Data Analysis for Chemistry*. Oxford: Oxford University Press.
3. Topping, J. (1984) *Errors of Observation and Their Treatment* (IV Edition). London: Chapman Hall.

Reference Books:

1. Harris, D. C. (2007). *Quantitative Chemical Analysis* (VII Edition). New York: W. H. Freeman and Company.
2. Levie, R. D. (2001). *How to Use Excel in Analytical Chemistry and in General Scientific Data Analysis*. Cambridge: Cambridge University Press.

3. IUPAC–IPCS. (1992). *Chemical Safety Matters*. Cambridge: Cambridge University Press.

ELECTIVE-II **Semester - II**

16CHP205B ANALYTICAL CHEMISTRY 4H 4C

Instruction Hours/week:L: 4 T:0 P:0 Marks: Internal:40 External: 60 Total:100

Course objectives

This course enables the students

- To learn about quantitative inorganic analysis.
- To understand the different colorimetric analysis.
- To learn about electrochemical methods of analysis.
- To learn different chromatographic techniques.
- To understand how to analyze the data obtained.
- To Explain about various analytical techniques for inorganic compounds.

Course Outcomes (CO's)

On successful completion of the course the students should have to

1. Learned about quantitative inorganic analysis.
2. Understood the different colorimetric analysis.
3. Learned the electrochemical methods of analysis.
4. Understood the different chromatographic techniques.
5. Learned about how to analyze the data obtained.
6. Explained the various analytical techniques for inorganic compounds.

Methodology

Blackboard teaching, Powerpoint presentation and group discussion.

UNIT-I

Quantitative Inorganic Analysis: Theoretical basis of quantitative inorganic analysis-common ion effect solubility product, effect of acid, temperature and solvent upon the solubility of a precipitate.

Supersaturation-Von Weimarn concept. Formation and treatment of precipitates-co-precipitation and post-precipitation. Precipitation from homogeneous solution. Specific and selective precipitants.

Principles of acid-base, oxidation-reduction, precipitation and complexometric titrations-indicators used in such titrations. Uses of organic reagents in inorganic quantitative and qualitative analysis.

UNIT-II

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

UNIT-III

Techniques in Inorganic Chemistry: Colorimetry: Theoretical and practical aspects of colorimetric analysis. Flame emission and atomic absorption spectroscopy – types of atomic spectroscopy – emission methods – absorption methods – fluorescence methods –

source and atomizers for atomic spectroscopy – flame atomizers – eletrothermal atomizers – principle and applications of atomic absorption spectroscopy. Advantages of atomic absorption spectrometry over flame photometry.

UNIT-IV

Electrochemical Methods of Analysis: Cyclic votammetry, coulometry and amperometry-principle and applications.

Thermal characterization techniques: Principle and applications of differential thermal analysis (DTA), differentials scanning calorimetry (DSC) and thermogravimetric analysis (TGA) thermometric titration.

UNIT- V

Chromatographic Methods: Classification – techniques and applications in column, size-exclusion, ion exchange, paper and thin layer chromatography.
Gas chromatography and high performance liquid chromatography (HPLC)-principle, equipment design, sample injection system, columns, detectors and applications.

SUGGESTED READINGS:

Text Books:

1. Svehla, G. (2002). *Vogel's Qualitative Inorganic Analysis* (VII Edition). Singapore: Pearson Education.
2. Christian, G. D. (2007). *Analytical Chemistry* (VI Edition). United States: John Wiley & Sons.
3. Skoog, D. A., West, D. M., Holler, F. J., & Crouch, S. R. (2014). *Fundamentals of Analytical Chemistry* (IX Edition). United States of America: Cengage Learning.

Reference Books:

1. Skoog, D. A., Holler, F. J., & Crouch, S. R. (2007). *Principles of Instrumental Analysis* (VI Edition). United States of America: Thomson Brooks/Cole Publishers.

ELECTIVE-II **Semester - II**

16CHP205C ORGANOMETALLIC CHEMISTRY 4H 4C

Instruction Hours/week:L: 4 T:0 P:0 Marks: Internal:40 External: 60 Total:100

Course objectives

This course enables the students

- To learn about nature of the bonding between organic ligands and metals.
- To understand about the metal alkyl complexes.
- To learn about the alkene and cyclopentadienyl complexes.
- To understand about the usage of organometallic compounds as catalysts
- To learn about the organometallic compound used as the catalyst in hydrogenation and hydroxylation of olefins.
- To study the concept of oxidation and polymerization of olefins.

Course Outcomes

On the completion of the course

1. Learned about the Alkyls and Arene complexes
2. Understood the bonding in olefin, acetylene and allyl systems
3. Known about the concepts of synthesis, structure and bonding in metallocenes
4. Understood the Organometallic reaction mechanisms and its applications
5. Learned about the Catalysis, hydrogenation of olefins and oxoprocess
6. Studied the concept of oxidation of olefins and polymerization

Methodology

Blackboard teaching, Powerpoint presentation and group discussion.

UNIT- I

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

UNIT- II

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

UNIT- III

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

UNIT- IV

Cyclopentadienyl complexes: Metallocenes - synthesis of metallocenes - bonding in metallocenes - reactions of metallocenes - Cp_2Fe/Cp_2Fe+ couples in biosensors - bent sandwich complexes - bonding in bent sandwich complexes - metallocene halides and hydrides - metallocene and stereospecific polymerisation of 1-alkenes - cyclopentadiene as a non-spectator ligand - monocyclopentadienyl (half-sandwich) complexes - synthesis and structures of allyl complexes - arene complexes - synthesis - structure and reactivity of arene complexes - multidecker complexes.

UNIT - V

Organometallic compounds in homogeneous catalytic reactions: Coordinative unsaturation - acid-base behaviour reaction - migration of atoms or groups from metal to ligand - insertion reaction - reactions of coordinated ligands - catalytic reactions of alkenes - isomerisation of alkenes - hydrogenation - hydroformylation and hydrosilation of alkenes - alkene polymerisation and oligomerisation - fluxional molecules.

SUGGESTED READINGS:

Text Books:

1. Huheey, J. E., Keitler, E. A., & Keitler, R. L. (2002). *Inorganic Chemistry-Principles of Structure and Reactivity* (IV Edition). Singapore: Pearson Education.
2. Haiduc, I., & Zuckerman, J. J. (2011). *Basic Organometallic Chemistry*. Brelin: Walter de Gruyter.

Reference Books:

1. Bockmann, M. (1996). *Organometallics 1- Complexes with transition metal-carbon-bonds*. UK: Oxford science publications.
2. Bockmann, M. (1996). *Organometallics 2- Complexes with transition metal-carbon bonds*. UK: Oxford science publications.
3. Cotton, F. A., & Wilkinson, G. (1978). *Basic Inorganic Chemistry*. Wiley Easter.

Semester - II

16CHP211 INORGANIC CHEMISTRY PRACTICAL–I 4H 2C
(QUALITATIVE ANALYSIS AND PREPARATIONS)

Instruction Hours/week:L: 0 T:0 P:4 Marks: Internal:40 External: 60 Total:100

Course Objectives

The course enables the students should have

- To learn about the qualitative analysis by semi micro-qualitative analysis method.
- To learn the preparation of inorganic complexes.
- To describe the basic concept and advantages of semi- micro qualitative analysis.
- To understand the systematic separation d-block elements
- To study the step wise procedure to predict the anions along with metals
- To identify the d-block elements with their special tests.

Course Outcomes

Students have to,

1. Learned about the qualitative analysis by semi micro-qualitative analysis method.
2. Learned the preparation of inorganic complexes.
3. Described the basic concept and advantages of semi- micro qualitative analysis.
4. Understood the systematic separation d-block elements
5. Studied the step wise procedure to predict the anions along with metals
6. Identified the d-block elements with their special tests.

Methodology

Blackboard teaching and Demonstration.

Contents

Thallium, Tungsten, Selenium, Tellurium, Molybdenum, Cerium, Thorium, Titanium, Zirconium, Vanadium, Beryllium, Uranium and Lithium.

Note: Each student should analyze a minimum of six inorganic mixtures.

About ten preparations involving different techniques selected from the following:

Lead tetra acetate, dipyridinium hexaplumbate, hydroxylamine hydrochloride, ortho and para- hydroxy phenyl mercuric chloride, potassium cupric chloride, chrome alum, copperI chloride, tris(thio urea) copper(I) Chloride, potassium trioxalato- aluminato(III), potassium trioxalato-chromate(III), potassium trioxalato- ferrate(III), hexammine cobalt(III)chloride, chloropentammine chromium(III), chloro aquo pentammine chromium(III) nitrate, tetrammine copper(II) sulphate, ammonium hexa chloro stanate(IV).

Note: Each student should do a minimum of ten preparations.

SUGGESTED READINGS:

Text Books:

1. Ramanujam, V. V. (2004). *Inorganic Semi-micro Qualitative Analysis* (III Edition). Chennai: The National Publishing Company.
2. Venkateswaran, V., Veeraswamy, R., & Kulandaivelu, A. R. (2004). *Basic Principles of Practical Chemistry* (II Edition). New Delhi: S. Chand Publications.
3. Siddhiqui, Z. N. (2002). *Practical Industrial Chemistry* (I Edition). New Delhi: Anmol Publications Pvt. Ltd.

Reference Books:

1. Mendham, J. R., Denney, C., Barnes, J. D., & Thomas, M. (2002). *Vogel's Textbook of Quantitative Chemical Analysis* (VI Edition). Singapore: Pearson Education Ltd.
2. Lepse, P. A., & Peter, L. B. (1986). *Lab Manual for Lingren's Essentials of Chemistry*. New Delhi: Prentice Hall.

Semester - II

16CHP212 INORGANIC CHEMISTRY PRACTICAL –II 4H 2C
(QUANTITATIVE ANALYSIS AND COMPLEX PREPARATIONS)

Instruction Hours/week:L: 0 T:0 P:4 Marks: Internal:40 External: 60 Total:100

Course Objectives

Course enables the students should have

- To learn about the basic principles about quantitative analyses.
- To study the concepts and systematic procedure in gravimetric analysis.
- To must know about the systematic procedure for estimation.
- To describe the synthesis method for in-organic co-ordination complexes
- To separate the molecules and identify its nature through chromatography technique.
- To apply this ideas and concepts to water treatment process, food science and forensic fields.

Course Outcomes

On successful completion of the course the students should have

1. Learned about the basic principles about quantitative analyses.
2. Studied the concepts and systematic procedure in gravimetric analysis.
3. Knew about the systematic procedure for estimation.
4. Described the synthesis method for in-organic co-ordination complexes
5. Known about separate the molecules and identify its nature through chromatography technique.
6. Applied this ideas and concepts to water treatment process, food science and forensic fields.

Methodology

Blackboard teaching and Demonstration.

Contents

- Analysis of mixture of ions – volumetry and gravimetry. Any four Complexometric titration- estimation of zinc, nickel, magnesium and calcium ions using Eriochrome black-T or muroxide indicator.
- Titrimetry: Oxidation using ceric and vanadium salts.
- Chromatography: Column, Paper and Thin layer chromatography.
- Titrations in non aqueous solvents.
- Preparation, analysis and study of co-ordination complexes (any 5).

SUGGESTED READINGS:

Text Books:

1. Lepse, P. A., & Peter, L. B. (1986). *Lab Manual for Lingren's Essentials of Chemistry*. New Delhi: Prentice Hall.
2. Mendham, J. R., Denney, C., Barnes, J. D., & Thomas, M. (2002). *Vogel's Textbook of Quantitative Chemical Analysis* (VI Edition). Singapore: Pearson Education Ltd.

3. Ramanujam, V. V. (2004). *Inorganic Semi-micro Qualitative Analysis* (III Edition). Chennai: The National Publishing Company.

Reference Books:

1. Siddhiqui, Z. N. (2002). *Practical Industrial Chemistry* (I Edition). New Delhi: Anmol Publications Pvt. Ltd.
2. Venkateswaran, V., Veeraswamy, R., & Kulandaivelu, A. R. (2004). *Basic Principles of Practical Chemistry* (II Edition). New Delhi: S. Chand Publications.

Semester-III

16CHP301 ORGANIC CHEMISTRY- III 4H 4C
(NATURAL PRODUCTS)

Instruction Hours/week:L: 4 T:0 P:0 Marks: Internal:40 External: 60 Total:100

Course Objectives

On successful completion of the course the students should have,

- To Study about Isolation, classification and structure determination of simple terpenoids.
- To learn about Isolation, classification and structure determination of simple steroids and alkaloids
- To know the structure of proteins, enzymes and nucleic acids.
- To discuss about the biological application of DNA and RNA.
- To list the various reagents used in organic synthesis
- To apply this fundamentals to clarify the pharmacological and biological activity of organic molecules

Course outcomes

The students have

1. Studied about Isolation, classification and structure determination of simple terpenoids.
2. Learned about Isolation, classification and structure determination of simple steroids and alkaloids
3. Knew the structure of proteins, enzymes and nucleic acids.
4. Discussed about the biological application of DNA and RNA.
5. Remembered the various reagents used in organic synthesis
6. Applied this fundamentals to clarify the pharmacological and biological activity of organic molecules

Methodology

Blackboard teaching, Powerpoint presentation and group discussion.

UNIT-I

Terpenoids: Isolation and classification of terpenoids – general methods of determining structure of terpenoids –structural elucidation and synthesis of Zingiberene, Eudesmol, Abietic acid, Caryophyllene and Santonin-biosynthesis of monoterpenoids**.**

UNIT-II

Steroids: Introduction – structural elucidation and synthesis of Cholesterol (synthesis not necessary), Ergosterol, Vitamin D, Equilenin, Oestrone, Testosterone and Progesterone. Bile acids – biosynthesis of sterols.

UNIT-III

Alkaloids: Definition of an alkaloid-extraction of alkaloids-general properties - general methods of determining structure of alkaloids – structural elucidation and synthesis of Atropine, Morphine and Quinine -biosynthesis of quinoline alkaloids.

UNIT-IV

Proteins: General nature of proteins - classification of proteins – synthesis of peptides – oxytocin- insulin.

Enzymes: Nomenclature and classification - cofactors – specificity of enzyme action- mechanism of enzyme action. Nucleic acids- structures of RNA and DNA and their biological importance.

UNIT- V

Reagents in organic synthesis: Preparations and synthetic applications of DDQ, DBU, Dimethyl sulfoxide, trimethyl silyl iodide, Osmium tetroxide, Selenium dioxide, Dicyclohexylcarbodiimide (DCC), LDA, DIBAL-H and Mercuric acetate.

SUGGESTED READINGS:

Text Books:

1. Chatwal, G. R. (2011). *Organic Chemistry of Natural Products Vol. II*. New Delhi: Himalaya Publishing House.
2. Finar, I. L. (2000). *Organic Chemistry Vol. II: Stereochemistry and the Chemistry of Natural Products* (V Edition). New Delhi: Addison Wesley Longman (Singapore) Pvt. Ltd- Indian Branch.
3. Smith, M. B., & March, J. (2007). *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure* (VI Edition). New Jersey: John Wiley & Sons, Inc., Hoboken.

Reference Books:

1. Chatwal, G. R. (2011). *Organic Chemistry of Natural Products. Vol. I*. New Delhi: Himalaya Publishing House.
2. Sanyal, S. N. (2006). *Reactions, Rearrangements and Reagents* (IV Edition). New Delhi: Bharathi Bhawan (Publishers and Distributors).
3. Tewari, N. (2011). *Advanced Organic Reaction Mechanism* (III Edition). Kolkata: Books and Allied (P) Ltd.
4. Agarwal, O. P. (2004). *Natural Product Chemistry Vol. II*. Meerut: Goel Publishing House.

Semester-III

16CHP302 PHYSICAL CHEMISTRY- III (THERMODYNAMICS) 4H 4C

Instruction Hours/week:L: 4 T:0 P:0 Marks: Internal:40 External: 60 Total:100

Course Objectives

The course enables the student to

- Understand about thermodynamics and Non-ideal systems
- Learn the third law of thermodynamics
- Study the classical Maxwell-Boltzman and quantum statistics
- Know about partition functions and determining thermodynamic properties
- Understand heat capacity of solids.
- Apply the thermodynamic factors in various organic synthesis processes (how the reaction condition and reaction rate various depend on the thermodynamic factors).

Course Outcomes

The students have to,

1. Understood about thermodynamics and Non-ideal systems
2. Learned the third law of thermodynamics
3. Studied the classical Maxwell-Boltzman and quantum statistics
4. Knew about partition functions and determining thermodynamic properties
5. Understood heat capacity of solids.
6. Applied the thermodynamic factors in various organic synthesis processes (how the reaction condition and reaction rate various depend on the thermodynamic factors).

Methodology

Blackboard teaching, Powerpoint presentation and group discussion.

UNIT – I

Themodynamics and Non-ideal systems: Chemical potential and the definition of fugacity. Determination of fugacity of gases by graphical method and from equations of state. Variation of fugacity with temperature. Fugacity and the standard states for non ideal gases.

Definition of activity. Activity coefficient. Temperature coefficient of activity. Standard states. Applications of activity concept to solutions. The rational and practical approaches. Measurement of activity of solvent from colligative properties. Determination of activity of solute.

UNIT – II

Third Law of Thermodynamics: Probability and third law. Need for third law. Nernst heat theorem and other forms stating third law. Thermodynamic quantities at absolute zero. Statistical meaning of third law and apparent exception.

Mathematical Introduction: Theories of permutation & combination, laws of probability. Distribution laws. Gaussian distribution.

UNIT – III

Classical Maxwell – Boltzmann Statistics: Maxwell distribution law for molecular velocities and molecular speeds in an ideal gas. Velocity and speed distribution functions. Experimental verification of Maxwell distribution law. Evaluation of average speed, root mean square speed and most probable speed from distribution law. Distribution function in terms of the kinetic energy of an ideal gas. The principle of equipartition of energy and the calculation of heat capacities of ideal gases. Limitations of the principle of equipartition of energy.

Quantum statistics: Maxwell-Boltzmann statistics. Thermodynamic probability. Thermodynamic probabilities of systems in equilibrium. Boltzmann expression for entropy. Stirling's approximation. State of maximum thermodynamics probability. Legrangian multipliers. Thermodynamic probabilities of systems involving energy levels. Maxwell-Boltzmann distribution law. Evaluation of alpha and beta in MB distribution law.

UNIT – IV

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

UNIT – V

Heat capacities of solids: Einstein's and Debye's theories of heat capacities of solids. Bose-Einstein and Fermi-Dirac Statistics: Bose Einstein distribution law- Entropy of Bose Einstein gas. Planck distribution law of black body radiation. Fermi-Dirac distribution law. Entropy of a Fermi-Dirac gas. Heat capacities of the electron gas and the heat capacities of metals. Negative absolute temperature.

SUGGESTED READINGS:

Text Books:

1. Glasstone, S. (2002). *Thermodynamics for Chemists*. New York: Litton Edition Publishing.
2. Atkins, P., & De Paula, J. (2014). *Atkins Physical Chemistry* (X Edition). Oxford: Oxford University Press.
3. Kapoor, K. L. (2005). *Text Book Physical Chemistry Vol. V*. New Delhi: MacMillan India Ltd.

Reference Books:

1. Lavin, I. N. (2002). *Physical Chemistry* (V Edition). New Delhi: Tata-McGraw Hill Publishing Company.
2. Whittakar, A. G. (2001). *Physical Chemistry*. New Delhi: Mount & Heal Viva Books Pvt. Ltd.

Semester -III

16CHP303 PHYSICAL METHODS IN CHEMISTRY (INSTRUMENTATION) 4H 4C

Instruction Hours/week:L: 4 T:0 P:0 Marks: Internal:40 External: 60 Total:100

Course Objectives

The course successfully enables the student,

- To understand different chromatographic methods.
- To discuss about electron spectroscopy and thermal analysis
- To learn Circular Dichroism and Optical Rotatory Dispersion
- To describe the Electron Spin Resonance spectroscopy
- To know about flame emission spectroscopy.
- To apply the chromatographic and spectroscopic concepts for separation and identification of mixture compounds/complex/metals.

Course outcomes

The students have to

1. Understood different chromatographic methods.
2. Discussed about electron spectroscopy and thermal analysis
3. Learned Circular Dichroism and Optical Rotatory Dispersion
4. Described the Electron Spin Resonance spectroscopy
5. Knew about flame emission spectroscopy.
6. Applied the chromatographic and spectroscopic concepts for separation and identification of mixture compounds/complex/metals.

Methodology

Blackboard teaching, Powerpoint presentation and group discussion.

UNIT – I

Chromatography: Theory, instrumentation, basic principles & application in the chemical analysis of the following – columns, paper, thin layer and ion exchange-gel permeation-HPLC applications in chemical analysis-gas chromatography**.**

UNIT – II

Thermal analysis: Differential thermal analysis DTA and differential scanning calorimetry DSC - basic principles - thermo gravimetric analysis.

Electron spectroscopy: ESCA XPS: Principle, chemical shifts - description of ESCA spectrometer, X-ray sources, samples, analysis, detectors and recording devices-applications.

Auger electron spectroscopy AES and Ultra-Violet photo electron spectroscopy UPS/PES principles and applications.

UNIT – III

Circular Dichroism and Optical Rotatory Dispersion: Basic principles -cotton effects-octants rule –axial halo ketone rule-application of ORD and CD. Tyndal Scattering-turbidimetry and nephelometry-applications. Atomic absorption spectroscopy.

UNIT – IV

ESR spectroscopy: Theory - derivative curves - g shift - hyperfine splitting-isotropic and anisotropic systems-zero field splitting and Kramer degeneracy. Identification of free radicals – applications to copper complexes.

UNIT – V

Flame Emission Spectroscopy: Introduction, flames and flame spectra, flames temperature, chemical reaction in flame and flame background. Flame photometers, Flame spectrophotometers, photosensitive detectors, single beam and double beam instruments, calibration curve, errors in flame photometers, applications.

SUGGESTED READINGS:

Text Books:

1. Gopalan, V., Subramanian, P. S., & Rangarajan, K. (2003). *Elements of Analytical Chemistry*. New Delhi: S. Chand and Sons.
2. Usharani, S. (2002). *Analytical Chemistry*. Chennai: MacMillan India Ltd.
3. Sharma, B. K. (2005). *Instrumental Methods of Chemical Analysis* (24th Edition). Meerut: Krishna Prakashan Media (P) Ltd.
4. Ewing, G. W. (1988). *Instrumental Methods of Chemical Analysis* (III Edition). Singapore: McGraw Hill International Edition.

Reference Books:

1. Chatwal, G. R., & Anand, S. K. (2015). *Instrumental Methods of Chemical Analysis* (V Edition). New Delhi: Himalaya Publishing House.
2. Drago, R .S. (1965). *Physical Methods in Inorganic Chemistry*. New York: Reinhold Publishing Corporation.
3. Skoog, D. A., & West, D. M. (2004). *Fundamentals of Analytical Chemistry* (VIII Edition). Singapore: Thomson Book Store.
4. Svehla, G. (2002). *Vogel's Qualitative Inorganic Analysis* (VII Edition). Singapore. Pearson Education

Semester–III

16CHP304 NANOCHEMISTRY 4H 4C

Instruction Hours/week:L: 4 T:0 P:0 Marks: Internal:40 External: 60 Total:100

Course Objectives

The course enables the student

- To know the history and perspectives of Nanotechnology.
- To learn about the various types and significant of 1D, 2D and 3D nanoparticles
- To list the various types of nanoparticles and its application.
- To discuss about carbon based nanomaterials and its properties
- To explain the metal oxide based nano materials
- To motivate and lead the student in the field of nanotechnology.

Course Outcomes

The completion of this course, students

1. Knew about the history and perspectives of Nanotechnology.
2. Learned about the various types and significant of 1D, 2D and 3D nanoparticles
3. Remembered the various types of nanoparticles and its application.
4. Discussed about carbon based nanomaterials and its properties
5. Explained the metal oxide based nano materials
6. Motivated and lead them in the pathway of nanotechnology

Methodology

Blackboard teaching, Powerpoint presentation and group discussion.

UNIT I: Introduction: History scope and perspectives of nano-chemistry

UNIT II: Synthesis and stabilization of nanoparticles, chemical reduction; reactions in micelles, emulsions, and dendrimers; photochemical and radiation chemical reduction; cryochemical synthesis: Physical methods, particles of various shapes and films.

UNIT III: Experimental techniques: Electron microscopy: Transmission electron microscopy: probe
Microscopy: Probe microscopy: diffraction techniques X-ray diffraction, neutron diffraction: Miscellaneous
Techniques, comparison of spectral techniques used for elemental analysis

UNIT IV: Size effects in nanochemistry: Models of reactions of metal atoms in matrices; properties;
Kinetic peculiarities of chemical processes on the surface of nanoparticles; Thermodynamic features of nanoparticles.

UNIT V: Applications of nanoparticle in various fundamental research, industries, medical field and environmental issue; toxicity, biosafety and ethical issue in application of nanoparticle

SUGGESTED READINGS:

Text Books:

1. Br'echignac, C., Houdy., & Lahmani, M. (2007). *Nanomaterials and Nanochemistry*. New York: Springer Berlin Heidelberg.
1. Hosokawa, M., Nogi, K., Naito, M., & Yokoyama, T. (2012). *Nanoparticle Technology Handbook* (II Edition). Elsevier.

Reference Books:

1. Theodore, L. (2006). *Nanotechnology: Basic Calculations for Engineers and Scientists*. Hoboken: John Wiley & Sons. Inc., Publication.

ELECTIVE-III **Semester-III**

16CHP305A **POLYMER CHEMISTRY** **4H 4C**

Instruction Hours/week:L: 4 T:0 P:0 Marks: Internal:40 External: 60 Total:100

Course Objectives

The course enables the student

- To study about the basic concepts of polymerization.
- To explains the coordination polymerization and apply the Ziegler-natta catalyst in polymer synthesis.
- To understand the molecular weight determination methods of the polymer and apply it identifies the polymer properties.
- To discuss about the polymer processing and properties of commercial polymers
- To apply the polymer processing technique to prepare the polymer products
- To list out the commercial polymers and its application

Course outcomes

The students have

1. Studied about the basic concepts of polymerization.
2. Explained the coordination polymerization and apply the Ziegler-natta catalyst in polymer synthesis.
3. Understood the molecular weight determination methods of the polymer and apply it identifies the polymer properties.
4. Discussed about the polymer processing and properties of commercial polymers
5. Applied the polymer processing technique to prepare the polymer products
6. Remembered the commercial polymers and its application

Methodology

Blackboard teaching, Powerpoint presentation and group discussion.

UNIT – I

Polymer Basic Concepts: Monomers, repeat units, degree of polymerization, linear, branched and network polymers. Condensation polymerization: Mechanism of stepwise polymerization. Kinetics and statistics of linear stepwise polymerization. Addition polymerization: Free radical, cationic and anionic polymerization. Polymerization conditions. Polymerization in homogeneous and heterogeneous systems.

UNIT – II

Co-ordination Polymerization: Kinetics, mono and bimetallic mechanism of co-ordination polymers. Zeigler Natta catalyst, co-polymerization: Block and graft co-polymers, kinetics of copolymerization. Types of co-polymerization. Reactivity ratio.

UNIT–III

Molecular Weight and Properties: Polydispersion – average molecular weight concept, number, weight and viscosity average molecular weights. Measurement of molecular weights. Viscosity, light scattering, osmotic and ultracentrifugation methods. Polymer

structure and physical properties – crystalline melting point T_m. The glass transition temperature. Determination of T_g. Relationship between T_m and T_g.

UNIT – IV

Polymer Processing: Plastics, elastomers and fibres. Compounding, processing techniques: calendering, die casting, rotational casting, film casting, injection moulding, blow moulding extrusion, moulding, thermoforming, foaming, reinforcing and fibre spinning.

UNIT – V

Properties of Commercial Polymers: Polyethylene, polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins and silicone polymers. Functional polymers, fire retarding polymers and electrically conducting polymers. Biomedical polymers – contact lens, dental polymers, artificial heart, kidney, skin and blood cells.

SUGGESTED READINGS:

Text Books:

1. Billmeyer, F. W. (2003). *Text Book of Polymer Science* (III Edition). New York: John Wiley.
2. Gowariker, V. R., Viswanathan, N. V., & Sreedhar, J. (2015). *Polymer Science* (II Edition). New Delhi: New Age International Private Ltd.
3. Alcock, H. R., Lampe, F. W., & Mark, J. E. (2003). *Contemporary Polymer Chemistry* (III Edition). NJ: Prentice Hall. Englewood Cliffs.

Reference Books:

1. Flory, P. J. (1953). *Principles of Polymer Chemistry*. New York: Cornell University Press.
2. Odian, G. (2004). *Principles of Polymerization* (IV Edition). New York: John Wiley & Sons.

ELECTIVE-III **Semester-III**

16CHP305B **TEXTILE CHEMISTRY** **4H 4C**

Instruction Hours/week:L: 4 T:0 P:0 Marks: Internal:40 External: 60 Total:100

Course Objectives

The course enables the student

- To understand about the classification, Chemical structure, production, properties and uses of fibers.
- To learn about the dyeing process on fibers.
- To discuss the classification of dyes
- To learn the Pollution Control in Textile Industry.
- To explain the various finishing process of fibers.
- To apply this fundamentals to fabricate the material and its dying process.

Course outcomes

On the successful completion of this course, Students

1. Understood about the classification, Chemical structure, production, properties and uses of fibers.
2. Learned about the dyeing process on fibers.
3. Discussed the classification of dyes
4. Learned the Pollution Control in Textile Industry.
5. Explained the various finishing process of fibers.
6. Applied these fundamentals to fabricate the material and its dying process.

Methodology

Blackboard teaching, Powerpoint presentation and group discussion.

UNIT- I

Fibres: General classification of fibres-chemical structure, production, properties and uses of the following natural fibres (a) natural cellulose fibres (cotton and jute) (b) natural protein fibre (wool and silk).

Chemical structure, production, properties and uses of the following synthetic fibres. (i) Man made cellulosic fibres (Rayon, modified cellulose fibres) (ii) Polyamide fibres (different types of nylons) (iii) Poly ester fibres.

UNIT- II

Dyeing Process: Impurities in raw cotton and grey cloth, wool and silk- general principles of the removal – scouring – bleaching – desizing – kierboiling- chemicking.

Dyeing - Dyeing of wool and silk –fastness properties of dyed materials – dyeing of nylon, terylene and other synthetic fibres.

UNIT- III

Finishing: Finishes given to fabrics- mechanical finishes on cotton, wool and silk, method used in process of mercerizing –anti-crease and anti-shrink finishes –water proofing.

UNIT-IV

Types of Dyes: Quinonoid dyes-examples and structure-Anthroquinone and Mordant dyes-synthesis and applications of Alizarin-Phthalocyanin dyes-Copper Phthalocyanin-synthesis and applications.

Diphenylmethane dyes- Auramine-Triphenylmethane dyes-Malachite green, Crystal violet, Pararosaniline-preparation and applications.

Indigo dyes-preparation and application-derivatives of Indigo- synthesis and uses of Indigosol and tetrahaloindigo.

Phthalein dyes-Phenolphthalein- preparation and applications.

Xanthene dyes-Rhodamine B, Fluorescein-Eosin- preparation and applications.

UNIT-V

Pollution Control in Textile Industry: Textile effluent-characteristics, effect of untreated effluent, degradability of wastes. Effluent treatment plants-aerated lagoon, photo oxidation process.

SUGGESTED READINGS:

Text Books:

1. Chatwal, R. (1995). *Synthetic Dyes*. Mumbai: Himalayan Publishing House.
2. Sadov, F., & Horchagin, M. (1978). *Chemical Technology of Fibrous Materials-A.* Matetshy. U.S.A: Mir Publishers Easton's Books. Inc. Mount Vernon.
3. Joseph, M. L., Hudson, P. B., Clapp, A. C., & Kness, D. (1993). *Joseph's Introductory Textile Science* (VI Edition). Fort Worth: Harcourt Brace Jovanovich College Publishers.
4. Luniak, B. (1953). *The Identification of Textile Fibres: The Identification of Textile Fibres: Qualitative and Quantitative Analysis of Fibre Blends*. London: Pitman Publisher.

Reference Books:

1. Sharma, B. K. (1997). Industrial *Chemistry*. New Delhi: Goel Publishing Co.
2. Prayag. R. S. (1989). *Dyeing of Wool, Silk and Manmade Fibres*. Dharwad: Noves Data Corporation.
3. Shenai. V. A. (1973). *Chemistry of Dyes and Principles of Dyeing*. Bombay: Sevak Publication.

ELECTIVE-III **Semester - II**

16CHP305C INDUSTRIAL CHEMISTRY 4H 4C

(APPLIED BIOINORGANIC CHEMISTRY, INORGANIC DRUG TARGETS AND METALS IN MEDICINE)

Instruction Hours/week:L: 4 T:0 P:0 Marks: Internal:40 External: 60 Total:100

Course Objectives

This course enables the students

- To give the knowledge of the role of metals in human body
- To learn about the physical methods in bioinorganic chemistry, metal biomolecules interactions, complexes, and drug discovery.
- To give knowledge in Binding of Metal Ions and Complexes to Biomolecules
- To Learn about complexes and chelating agents
- To Provide fundamental knowledge in Drug Discovery and Design
- To apply these parameters to discover new pharmacokinetic molecules.

Course Outcomes

On the completion of this course, student should

1. Knew the knowledge of the role of metals in human body
2. Learned about the physical methods in bioinorganic chemistry, metal biomolecules interactions, complexes, and drug discovery.
3. Understood the knowledge in Binding of Metal Ions and Complexes to Biomolecules
4. Learned about complexes and chelating agents
5. Provided the fundamental knowledge in Drug Discovery and Design
6. Applied these parameters to discover new pharmacokinetic molecules.

Methodology

Blackboard teaching, Powerpoint presentation and group discussion.

UNIT- I

Metals in the Human Body: General principles - the elements in the human body - biological significance, storage and transport of Fe, Zn, Cu, Mo, Co, Cr, V and Ni - metal functions in metalloproteins -metallo enzyme functions -supplying elements to the body - metals and human health.

UNIT- II

Physical Methods in Bioinorganic Chemistry: X-ray methods - magnetic resonance methods - mossbauer spectroscopy - magnetic measurements -other instrumental methods -atomic force microscopy - fast and time-resolved methods - stopped-flow kinetic methods - flash photolysis - time-resolved crystallography.

UNIT- III

Binding of Metal Ions and Complexes to Biomolecules: Nucleic acid structures - fundamental interactions with nucleic acids - binding interactions of tris(phenanthroline) metal complexes with DNA - techniques to monitor binding - applications of metal complexes that bind to nucleic acids -biopolymer promoted metal ligand interactions.

UNIT- IV

Complexes and Cheating Agents: Labile and inert complexes - metal-ligand selectivity-HSAB approach-chelate effect and Irving-William series -survey of metals used for diagnosis and chemotherapy-radiodiagnostic agents-Magnetic Resonance Imaging (MRI) - gold and other metal phosphines-main-group and transition metal compounds - miscellaneous metals in medicine-chelating agents and therapy - EDTA-evolution, chemical properties, *in vivo* chelation of radionuclides, dosage and toxicity .

UNIT-V

Drug Discovery and Design: Outline- therapeutic index, chemotherapeutic index, structure- activity relationship (SAR) and quantitative structure-activity relationship (QSAR)- Factors governing drug design- computer aided drug design-cancer chemotherapy-bioinorganic chemistry (DNA binding) of platinum anticancer drugs (cisplatin and carboplatin)-mechanism of action studies-clinical trials and their significance- production and quality control- patent protection.

SUGGESTED READINGS:

Text Books:

1. Taylor, D. M., & Williams, D. R. (1995). *Trace Element Medicine and Chelation Therapy* (I Edition). United Kingdom: The Royal Society of Chemistry.
2. Ashutosh Kar, (2000). *Medicinal Chemistry*. New Delhi: New Age International Publishers.
3. Gareth Thomas, (2000). *Medicinal Chemistry*. United Kingdom: John-Wiley & Sons Ltd.

Reference Books:

1. Bertini, I., Gray, H. B., Lippard, S. J., & Valentine, J. S. (1994). *Bioinorganic Chemistry*. California: University Science books.
2. Roat-Malone, R. M. (2002). *Bioinorganic Chemistry*. NJ: John Wiley & Sons. Inc.

Semester-III

16CHP311 PHYSICAL CHEMISTRY PRACTICAL -I 4H 2C

(MOLECULAR WEIGHT DETERMINATION AND CONDUCTOMETRIC TITRATIONS)

Instruction Hours/week:L: 0 T:0 P:4 Marks: Internal:40 External: 60 Total:100

Course Objectives

This course enables the students should have

- To Learn about the heat of solution, determination of molecular weight and distribution coefficient
- To study about basic concepts of conductometric titrations.
- To understand the various laws in electrochemistry.
- To apply the conductometric method for the solutions and measure its conductivity
- To know about how to handle the conductivity meter, spectrophotometer.
- To may realize the how distribution co-efficient influence the solubility of various systems.

Course Outcomes

On the completion of this course, students

1. Learned about the heat of solution, determination of molecular weight and distribution coefficient
2. Studied about basic concepts of conductometric titrations.
3. Understood the various laws in electrochemistry.
4. Applied the conductometric method for the solutions and measure its conductivity
5. Knew about how to handle the conductivity meter, spectrophotometer.
6. Applied the knowledge to realize the how distribution co-efficient influence the solubility of various systems.

Methodology

Blackboard teaching and Demonstration.

Contents

Heat of solution from solubility.

Molecular weight determination by

i. Freezing point depression of solvents benzene and water by Beckmann method
ii. By Rast micro methods

Distribution of activity and activity co-efficient by freezing point method.

Distribution co-efficient and determination of equilibrium constant.

Conductivity experiments:

Determination of

i) Equivalent conductance of a strong electrolyte and verification of Debye-Huckel Onsager law.

ii) Verification of Ostwald dilution law and Kohlraush law for weak electrolytes.

Conductometric determination of pK_a of a weak acid.

Hydrolysis constant of aniline hydrochloride.

Determination of the solubility of a sparingly soluble salt.

Conductometric titrations:

Acid-base and precipitation titrations including mixture of halides.

SUGGESTED READINGS:

Text Books:

1. Lepse, P. A., & Lyle B. P., (1986). *Lab Manual for Lingren's Essentials of Chemistry*. New Delhi: Prentice Hall.
2. Pandey, O. P, Bajpai, D. N., & Giri, S. (2001). *Practical Chemistry* (VIII Edition). New Delhi: S. Chand Publications.
3. Santi Rajan Palit and Sadhan Kumar, (1971). *Practical Physical Chemistry* (I Edition). Calcutta: Joy Publishers.

Reference Books:

1. Siddhiqui, Z. N. (2002). *Practical Industrial Chemistry* (I Edition). New Delhi: Anmol Publications Pvt. Ltd.
2. Thomas, A.O, (2003). *Practical Chemistry*. Cannanore: Scientific Book Center.
3. Venkateswaran, V., Veeraswamy, R., & Kulandaivelu, A. R. (2004). *Basic Principles of Practical Chemistry* (II Edition). New Delhi: S. Chand Publications.

Semester-III

16CHP312 PHYSICAL CHEMISTRY PRACTICAL- II 4H 2C
(CHEMICAL KINETICS AND POTENTIOMETRIC TITRATIONS)

Instruction Hours/week:L: 0 T:0 P:4 Marks: Internal:40 External: 60 Total:100

Course Objectives

This course enables the students should have

- To learn about the principles of electrochemistry and determination EMF
- To understand about the basic needs of Chemical Kinetics and Potentiometric titrations.
- To study the principles about adsorption process.
- To know about how to handle the potentiometer, electrodes and spectrophotometer.
- To apply the knowledge of chemical kinetics in various preparation organic/inorganic compounds.
- To investigate the metal concentration in water samples using adsorption technique.

Course Outcomes

On the completion of this course, students to

1. Learned about the principles of electrochemistry and determination EMF
2. Understood about the basic needs of Chemical Kinetics and Potentiometric titrations.
3. Studied the principles about adsorption process.
4. Knew about how to handle the potentiometer, electrodes and spectrophotometers.
5. Appling the knowledge of chemical kinetics in various preparation organic/inorganic compounds.
6. Investigating the metal concentration in water samples using adsorption technique.

Objectives

On successful completion of the course the students should have

(i) Learnt about the Chemical Kinetics and Potenciometric titrations.
(ii) Learnt the Principles of Adsorption experiments.

Methodology

Blackboard teaching and Demonstration.

Contents

Electromotive force determination of standard potentials of Cu, Zn and Ag.

Determination of pH and pKa values using hydrogen and quinhydrone electrodes and glass electrode pH meter- potentiometric acid-base titrations.

Determination of formal redox potential of a redox system and redox titrations.

Determination of solubility product of a sparingly soluble salt concentration cell and chemical cell.

Determination of activity co-efficients from emf data.

Precipitation titration of a mixture of halides.

Chemical kinetics:

i . Evaluation of Arrhenius parameters using acid hydrolysis of an ester.
ii. Base catalysed hydrolysis of an ester conductometrically.
iii. Rate of reaction between persulphate and iodide ions study of salt over the persulphate- iodide reaction.

Evaluation of catalytic constants for weak acids and verification of Bronsted catalysis law.

Adsorption Experiments:

Adsorption of oxalic acid and acetic acid on activated charcoal-Fruendlich isotherm.

SUGGESTED READINGS:

Text Books:

1. Lepse, P. A., & Lyle B. P., (1986). *Lab Manual for Lingren's Essentials of Chemistry*. New Delhi: Prentice Hall.
2. Pandey, O. P, Bajpai, D. N., & Giri, S. (2001). *Practical Chemistry* (VIII Edition). New Delhi: S. Chand Publications.
3. Santi Rajan Palit and Sadhan Kumar, (1971). *Practical Physical Chemistry* (I Edition). Calcutta: Joy Publishers.

Reference Books:

1. Siddhiqui, Z. N. (2002). *Practical Industrial Chemistry* (I Edition). New Delhi: Anmol Publications Pvt. Ltd.
2. Thomas, A.O, (2003). *Practical Chemistry*. Cannanore: Scientific Book Center.
3. Venkateswaran, V., Veeraswamy, R., & Kulandaivelu, A. R. (2004). *Basic Principles of Practical Chemistry* (II Edition). New Delhi: S. Chand Publications.

Semester-IV

16CHP491	**PROJECT WORK**	**30H 15C**

Instruction Hours/week: L:0 T:0 P:30 Marks: Internal: 40 External: 60 Total:100