Sri Sai University, Palampur

Syllabus for M.Sc. Chemistry

Choice Based Credit System (CBCS)

Course Effective from Academic Year 2022-23

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1. DURATION OF THE PROGRAMME

(a) The degree programme leading to the award of Master of Science (M.Sc.) in chemistry shall be of TWO years duration and include four continuous semesters under Choice Based Credit System (CBCS).

(b) The programme shall be completed in a maximum of four years (8 Semesters), consecutively, from the date of admission to the programme.

2. PROGRAMME STRUCTURE

(a) The syllabi for M.Sc. in Chemistry is drafted as per the UGC guidelines for Learning Outcomes based Curriculum Framework (LOCF) based approach with an aim to equip the students with knowledge, skill, values and attitude.

(b) Usually a course refers to a 'paper' and is a component of an academic programme.

(c) The programmes shall include:

(i) **Core Course**: A core course is a compulsory paper to be studied by all the students to complete the requirements for the postgraduate degree.

(ii) **Elective Course**: Elective course is 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.

1. *Discipline Specific Elective (DSE) Course*: Elective courses offered by the main discipline/subject of study is referred to as Discipline Specific Elective.
2. *Open Elective Course*: An elective course chosen generally from other discipline(s)/subject(s), with an intention to seek exposure is called a Generic Elective.

(iii) **Self Study/Skill Enhancement Courses/Value Added Courses:** These courses are not mandatory and are thus non credit courses**.** Their performance of students in these courses will be either be indicated as Satisfactory or Unsatisfactory.

(iv) **Ability Enhancement Courses:** These courses are mandatory for students as it enhances the ability of students in specific discipline.

(d) The number of credits is given in the form L:T:P, where L, T and P indicates lecture, tutorial and practical laboratory credits respectively. Each lecture credit corresponds to one lecture hour per week, each tutorial credit corresponds to one tutorial hour per week while each laboratory credit corresponds to two laboratory hours per week. For example, 4:0:2 credits indicate that the course has 4 lectures, no tutorial session and two laboratory hours each week.

(e) The total credit required to complete the programme shall be a minimum of **98 credits**. Students may pursue courses for additional credits on their own (please refer to "SRI SAI UNIVERSITY REGULATIONS FOR CHOICE BASED CREDIT SYSTEM FOR UNDER- GRADUATE COURSES, 2021").

(f) The detailed structure of courses under M.Sc. Chemistry Programme shall be:

Sl. No.	Details of Courses	Credits		
		Theory	Practical	TOTAL
I	**Core Courses** (12 Theory of 4 credits each + 9 Practical of 2 credits each+ 1 Seminar of 2 credits+ 8 credits for Project)	11 X4 = 44	9X 2 = 18 1X 2 = 02 1X 8 =8	72
II	**Elective Courses** (4 Credits) (**4 Courses**)			
	(a) Discipline Specific Elective Courses (EC) (**3 Courses**)	4 X 4 = 16	--------	16
	(b) Open Elective (OE) Courses	2x2=4	-	4
III	**Ability Enhancement/Self Study/Skill Enhancement/Value Added Courses (2 Courses)**			
	(a) Value Added Courses (VAC) (Non Credit) (**2 Courses**) (On satisfactory completion of Course "S" will be awarded, either wise 'US' will be awarded) (**Non Credit**)	-		0
	(b) Self Study/Skill Enhancement Courses (SEC)	-		-
	(c) **Ability Enhancement Courses (2 courses + 1 Practical)**	1 X 2 = 2 1 X 3 = 3	1 X 1 = 1	6
Grand Total Credit				**98**

Course Structure
M. Sc. Chemistry

Course Code	Title of Course	Marks				Credits			
		Theory	Practical	Internal Assessment	Total	L	T	P	Total
SEMESTER-I									
CHEM-CC- 411	Group Theory & Non-Aqueous Solvent	60	0	40	100	4	0	0	**4**
CHEM-CC- 412	Reaction Mechanism and Stereochemistry	60	0	40	100	4	0	0	**4**
CHEM-CC- 413	Spectroscopy & Kinetics	60	0	40	100	4	0	0	**4**
MATH-AE- 414(A) **OR** **BIOL-AE-414(B)**	Mathematics for Chemists OR Biology for Chemists	30	0	20	50	2	0	0	**2**
CA-AE-415	Computer for Chemists	60		40	100	3	0	0	**3**
CHEM-CC-416P	Inorganic Chemistry Practical-I	--	50	--	50	0	0	2	**2**
CHEM-CC-417P	Organic Chemistry Practical-I	--	50	--	50	0	0	2	**2**
CHEM-CC-418P	Physical Chemistry Practical-I	--	50	--	50	0	0	2	**2**
CA-AE-419P	Computer Practical	--	50	--	50	0	0	1	**1**

Note: The students, having B.Sc in Biology, will have to opt for MATH-AE-414(A), while the students with B.Sc in Mathematics will have to choose BIO-AE-414(B).

SEMESTER-II									
CHEM-CC-421	Metal Ligand Bonding & Magnatochemistry	60	0	40	100	4	0	0	**4**
CHEM-CC-422	Aromatic, Elimination and Pericyclic Reactions	60	0	40	100	4	0	0	**4**
CHEM-CC-423	Thermodynamics & Electrochemistry	60	0	40	100	4	0	0	**4**
CHEM-CC-424	Organic Spectroscopy and Photochemistry	60	0	40	100	4	0	0	4
CHEM-CC-425P	Inorganic Chemistry Practical-II	--	50	--	50	0	0	2	**2**
CHEM-CC-426P	Organic Chemistry Practical-II	--	50	--	50	0	0	2	**2**
CHEM-CC-427P	Physical Chemistry Practical-II	--	50	--	50	0	0	2	**2**
----------	**Open Course-I***	**30**	--	20	50	0	0	2	**2**

***Students will have to choose one open elective course from other departments.**

SEMESTER-III

CHEM-CC-431	Analytical & Nuclear chemistry	60	0	40	100	4	0	0	**4**
CHEM-CC-432	Statistical Thermodynamics and Basic Quantum Chemistry	60	0	40	100	4	0	0	**4**
RM-CC-022	Research Methodology	60	0	40	100	4	0	0	**4**
	Elective Courses [CHEM-EC-434 (Inorganic Special) /435 (Organic Special /436 (Physical Special]								
CHEM-EC-433	Bioinorganic And Reaction Mechanism	60	0	40	100	4	0	0	**4**
CHEM-EC-434	Natural Products	60	0	40	100	4	0	0	**4**
CHEM-EC-435	Surface Chemistry & Advanced Electrochemistry	60	0	40	100	4	0	0	**4**
CHEM-CC-436P	Inorganic Chemistry Practical-III	--	50	--	50	0	0	2	**2**
CHEM-CC-437P	Organic Chemistry Practical-III	--	50	--	50	0	0	2	**2**
CHEM-CC-438P	Physical Chemistry Practical-III	--	50	--	50	0	0	2	**2**
CHEM-CC-500	Seminar		50		50	0	0	2	**2**
-------	**Open Course-II***	30	--	**20**	**50**	**0**	**0**	**2**	**2**

Note: Students will have to choose one paper from elective courses CHEM-EC-434/435/436 depending upon their field of interest. Further, open elective course* should be chosen from other departments.

SEMESTER-IV

	Elective Courses (Inorganic Chemistry: CHEM-EC-442/443/444/445) (Organic Chemistry: CHEM-EC-446/447/448/449) (Physical Chemistry: CHEM-EC-450/451/452/453)								
CHEM-CC-441	Techniques of chemical analysis	60	0	40	100	4	0	0	**4**
CHEM-EC-442	Chemistry of Materials	60	0	40	100	4	0	0	**4**
CHEM-EC-443	Advanced Organometallics	60	0	40	100	4	0	0	**4**
CHEM-EC-444	Inorganic Spectroscopy	60	0	40	100	4	0	0	**4**
CHEM-EC-445	Catalysis and Green Chemistry	60	0	40	100	4	0	0	**4**
CHEM-EC-446	Synthetic Strategies	60	0	40	100	4	0	0	**4**
CHEM-EC-447	Medicinal Chemistry								
CHEM-EC-448	Polymer Chemistry	60	0	40	100	4	0	0	**4**
CHEM-EC-449	Organometallic and Heterocyclic Chemistry	60	0	40	100	4	0	0	**4**
CHEM-EC-450	Solid State Chemistry	60	0	40	100	4	0	0	**4**
CHEM-EC-451	Advanced Quantum Chemistry	60	0	40	100	4	0	0	**4**
CHEM-EC-452	Biophysical Chemistry	60	0	40	100	4	0	0	**4**
CHEM-EC-453	Chemistry of Macromolecules	60	0	40	100	4	0	0	**4**
CHEM-CC-501	**Research Project**	----	--	--	200	0	0	8	**8**

CC: Core Courses; EC: Elective Courses; AE: Ability Enhancement Courses; (P): Practical; CHEM: Chemistry; COMP: Computer; MATH: Mathematics; BIO: Biology

Note: Students will have to choose ANY THREE elective papers depending upon their field of interest.

Core Courses

SEMESTER-I

L	T	P	Credit
4	0	0	4

CHEM-CC-411: Group Theory & Non Aqueous Solvent

Course Objectives	The objective of this course is to teach the advanced symmetry concepts of chemical molecules and its applications and also develop interest to identify the axis, plane, center and point group, polarity, dipole moment, product of symmetry operation and use of organic reagents and solvents.
Course Outcomes	By the end of the course students will be able to: • Predicting geometries of simple molecules. • Use of group theory to recognize and assign symmetry characteristics to molecules and objects, and to predict the appearance of a molecule's vibrational spectra as a function of symmetry. • Use organic reagents experimentally.

DETAILED CONTENT

MODULE-I

Group theory: The concept of group, symmetry elements and symmetry operations, assignment of point groups to inorganic molecules, some general rules for multiplications of symmetry operations, multiplication tables for water and ammonia, representations (matrices, matrix representations for C_{2V} and C_{3V} point groups irreducible representations), character and character tables for C_{2V} and C_{3V} point groups. Applications of group theory to chemical bonding (hybrid orbitals for σ-bonding in different geometries and hybrid orbitals for π-bonding. Symmetries of molecular orbitals in BF_3, C_2H_4 and B_2H_6.

MODULE-II

Application of Group Theory in Vibrational Spectroscopy: A brief idea about Infrared and Raman scattering spectroscopy. Vibrational modes as basis of group representations w.r.t. SO_2, $POCl_3$, $PtCl_4^{2-}$ and RuO_4.Mutual exclusion principle, classification of vibrational modes (i.e. stretching and angle deformation vibrations w.r.t. SO_2, $POCl_3$ and $PtCl_4^{2-}$.

MODULE-III

Non-Aqueous Solvents: Factors justifying the need of non-aqueous solution chemistry and failure of water as a solvent. Solution chemistry of sulphuric acid: Physical properties, ionic self-dehydration in H_2SO_4, high electrical conductance in spite of high viscosity. Chemistry of H_2SO_4 as an acid, as an dehydrating agent, as an oxidizing agent, as an medium to carry out acid-base neutralization reaction and as a differentiating solvent. Liquid BrF_3: physical properties, solubilities in BrF_3, self-ionization, acid base neutralization reactions, solvolytic reactions and formation of transition metal fluorides. Chemistry of molten salts as non-aqueous solvents: solvent properties, solution of metals, complex formation, unreactivity of molten salts, low temperature molten salts.

MODULE-IV

Inorganic Hydrides: Classification, preparation, bonding and their applications. Transition metal compounds with bonds to hydrogen, carbonyl hydrides and hydride anions. Classification, nomenclature, Wade's rules,

preparation, structure and bonding in boron hydrides (boranes), carboranes, metalloboranes and metallocarboranes.

MODULE-V

Organic Reagents in Inorganic Chemistry: Chelation, factors determining the stability of chelates (effect of ring size, oxidation state of the metal, coordination number of the metal); Use of Dimethylglyoxime, EDTA,8-Hydroxyquinoline, 1,10-Phenanthroline, Thiosemicarbazones and Dithiazone.

Books recommended:

1. *Chemical applications of Group Theory - F.A.Cotton*
2. *Inorganic Chemistry - Durrant and Durrant*
3. *Symmetry in Chemistry- Jaffe and Orchin*
4. *Non-aqueous solvents - H. Sisler*
5. *Non-aqueous solvents - T.C.Waddington*
6. *Non-aqueous solvents - Logowsky*
7. *Advanced Inorganic Chemistry:Cotton& Wilkinson,Vth Edn.*
8. *Concise course in Inorganic Chemistry- J.D.Lee*
9. *Nature of Chemical Bond - L. Pauling*
10. *Chemistry of Elements - Greenwood and Earnshaw*
11. *Inorganic Chemistry - T. Moeller*
12. *Inorganic Chemistry - J.E.Huheey 3rd Edn.*
13. *Topics in Current Chemistry (Inorganic/Bio-Chemistry)-Vol. 64*
14. *A Text Book of Quantitative Inorganic Analysis- A.I. Vogel*

SEMESTER-I

L	T	P	Credit
4	0	0	4

CHEM-CC-412: Reaction Mechanism and Stereochemistry

Course Objectives	The objective of present course is to teach the students to predict the relationships between organic chemical structures and their reactivity; to learn the fundamental and advanced concepts in reaction mechanisms in organic chemistry along with the study of reaction mechanisms in various types of substitution reactions; to predict and account for the most commonly encountered reaction mechanisms in organic chemistry; to explain the basic concepts and terms involved in stereochemistry; and to describe stereochemical like chiral reagents and catalysts
Course Outcomes	At the end of the course, the student will be able • To study the various known reactive intermediate in organic synthesis • To predict the relationships between organic chemical structures and their reactivity. • To learn the fundamental and advanced concepts in reaction mechanisms in organic chemistry along with the study of reaction mechanisms in various types of substitution reactions. • To study the new methodologies for altering the reactivity patterns of reactive intermediates • To predict the product of various reactions by taking into consideration of the stereochemistry of reacting molecules. • To determine absolute configuration of organic by various rules and techniques.

DETAILED CONTENT

MODULE-I

Nature of Bonding in Organic Molecules: Delocalized chemical bonding: kinds of molecules with delocalized bond, cross- conjugation, resonance, pπ-dπ bonding (ylides). aromaticity: other systems containing aromatic sextet, aromatic systems with electron number other than six. Huckel rule, other aromatic compounds, hyperconjugation. Supramolecular chemistry: Introduction, bonding other than covalent bond. Addition compounds, Crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxenes and their applications.

MODULE-II

Stereochemistry: Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity in acylic and cyclohexane systems. Steric strain due to unavoidable crowding. Elements of symmetry: chirality, molecules with more than one chiral center, threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, optical activity due to chiral planes, optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape. Asymmetric synthesis: Principle and categories with specific examples of asymmetric synthesis including newer methods involving enzymatic and catalytic reactions, enantio and diastereoselective synthesis. Stereoselective reactions: Cyclopropanation, hydroboration, catalytic hydrogenation, and metal ammonia reduction, stereoselective synthesis of (-) ephedrine and (+) φ- ephedrine. Stereospecific reactions: Elimination of 2,3- dibromobutane densyl

chloride(1,2-diphenyl-1-chloroethane), SN^2 reactions at chiral carbon.

MODULE-III

Reaction Mechanism: Structure and Reactivity: Thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammonds postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates.

Effect of structure on reactivity: resonance and field effects, steric effect. Quantitative treatment: Hammett equation and linear free energy relationship, substituent and reaction constants, Taft equation. Methods of determining reaction mechanism.

MODULE-IV

Aliphatic Nucleophilic Substitution: The SN_2, SN_1, mixed SN_1 and SN_2, SET mechanisms & SNi mechanism. The neighboring group mechanism, neighboring group participation by π and σ bonds, anchimeric assistance. Non-classical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements-Wagner-Meerwein, Pinacol-Pinacolone and Demjanov ring expansion and ring contraction. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Esterification of carboxylic acid, transesterification, transetherification and preparation of inorganic esters. Phase-transfer catalysis, and ultrasound, ambident nucleophile, regioselectivity.

MODULE-V

I. **Aliphatic Electrophilic Substitution:** Bimolecular mechanisms- SE2 and SEi. The SE1 mechanism, electrophilic substitution accompanied by double bond shifts, halogenations of aldehydes, ketones, acids and acyl halides. Effect of substrates, leaving group and the solvent system on reactivity. Aliphatic diazonium coupling, acylation at aliphatic carbon, alkylation of alkene, Stork-enamine reactions.

II. **Free radical reactions:** Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighboring group assistance, reactivity in aliphatic and aromatic substrates at a bridgehead and attacking radicals. Effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Gomberg Bachmann reaction, Sandmeyer reaction, Hoffmann -Loffler- Freytag reaction, Hunsdiecker reaction.

Books recommended:

1. *Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.*
2. *Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Plenum.*
3. *A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.*
4. *Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University Press.*
5. *Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice Hall.*
6. *Modern Organic Reactions, H.O. House, Benjamin.*
7. *Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic and Professional.*
8. *Pericyclic Reactions, S.M. Mukherji, Macmillan, India.*
9. *Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan.*
10. *Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.*
11. *Stereochemistry of Organic Compounds, P.S. Kalsi, New Age International.*

SEMESTER-I

L	T	P	Credit
4	0	0	4

CHEM-CC-413: Spectroscopy & Kinetics

Course Objectives	The objective of this course is to equip students with the necessary chemical knowledge concerning the fundamentals in the basic areas of physical chemistry viz. Spectroscopy and chemical kinetics. Also, to impart knowledge of various spectroscopic techniques and their applications to enhance problem-solving skills of students through numerical problems.
Course Outcomes	At the end of this course student will be able to • Explain the principle and instrumentation of nuclear magnetic and electron spin resonance spectroscopy. Make Students aware of the fine structure of ESR absorption and Hyperfine structure. • Understand Principles and applications of Mossbauer spectroscopy. • Recognize spectroscopy in Microwave, IR and Raman Spectra. • Explain all types of complex reactions viz reversible, consecutive and chain reactions.Study of different theories viz. collision and transition state and their rates. • Explain the mechanism and principles of surface and fast reactions.

DETAILED CONTENT

MODULE - I

Spectroscopy I: Theory of nuclear magnetic resonance (NMR) phenomenon. Chemical shift and its measurement. The fine structure (spin - spin coupling). Factors influencing chemical - shift and spin-spin coupling. Non-first-order spectra. Relaxation phenomena in NMR: spin-spin and spin-lattice relaxation processes. Line-width and rate processes. The nuclear Overhauser effect. An introduction to Fourier Transform NMR (FTNMR). Theory of electron spin resonance (ESR) phenomenon, fine and hyperfine structure of ESR, zero-field splitting of ESR signal. Mapping of charge density on molecule (Mc Connell relation). Mossbauer spectroscopy: a brief introduction (isomer - shift, quadrupole interaction and magnetic hyperfine interaction).

MODULE - II

Spectroscopy II: Rotational spectra: moment of inertia and rotational spectra of rigid and non - rigid diatomic molecules, rotational spectra of symmetric - top molecules. Vibrational spectra: vibrational energy of diatomic molecules. Anharmonic oscillator, overtones and hot bands. Vibrational excitation effect, Stark effect. Diatomic vibrator - rotator (P, Q and R – branches of diatomic molecules). Rotational - vibrational spectra of symmetric - top molecules. Raman spectroscopy: qualitative quantum theory of Raman scattering. Rotational Raman spectra of linear and symmetric - top molecules. Vibrational Raman spectra and mutual exclusion principle.

MODULE - III

Kinetics of complex reactions: Reversible /opposing reactions, consecutive / successive reactions, simultaneous side/parallel reactions, chain/free radical reactions viz. thermal(H_2-Br_2) and photochemical H_2-Cl_2) reactions. Rice-Herzfeld mechanism of dissociation of organic molecules viz. dissociation of ethane, decomposition of acetaldehyde as 3/2 and 1/2 order reactions. Kinetics of polymerization (molecular and free radical mechanisms). Reaction rates and chemical equilibrium, principle of microscopic reversibility, activation energy and activated complex.

MODULE - IV

Theories of reaction rates: The kinetic theory of collisions, transition state theory, comparison of collisions and transition state theories in simple gas reactions, steric factor, transmission -coefficient, steady - state hypothesis / transient phase theory, Lindemann's theory of unimolecular reaction, the thermodynamic formulation of reaction rates.

MODULE - V

1.Surface Reactions: Mechanism of surface reactions, unimolecular and bimolecular surface reactions, Langmuir - Hinshelwood mechanism for gases only.

2.Fast Reaction in aqueous solutions: Study of fast reactions by stopped flow method (principle and theory). Absolute rate theory applied to fast reactions.

Books recommended:

1. *Chemical Kinetics: K.J. Laidler*
2. *Kinetics and Mechanism of Reaction Rates: A.Frost and G. Pearson.*
3. *Modern Chemical Kinetics: H. Eyring*
4. *Theories of Reaction Rates: K.J. Laidler, H. Eyring and S. Glasston*
5. *Fast Reactions: J.N. Bradly*
6. *Fast Reactions in Solutions: Caldin*
7. *Basic Principles of Spectroscopy: R. Chang*
8. *NMR and Chemistry: J.W. Akit*
9. *Introduction to Molecular Spectroscopy: G.M. Barrow*
10. *Physical Chemistry: P.W. Atkins*
11. *Fundamentals of Molecular Spectroscopy: C.N. Banwell*

SEMESTER-I

L	T	P	Credit
0	0	2	2

CHEM-CC-416P: In-organic Chemistry Practical-I

Course Objectives	The objective of this course is; to apply previous and current knowledge for performing experiment scientifically.
Course Outcomes	Students are able to: • Determine hardness of water of various water samples. • Estimate the percentage of chlorine in bleaching powder. • Estimate the percentage of calcium in hard water sample/ given sample. • Gravimetric analysis of the sample.

DETAILED CONTENT

1. **Volumetric Analysis:**

(a) **Potassium iodate titrations**: Determination of iodide, hydrazine, antimony(III) and arsenic (III)

(b) **Potassium bromate titrations**
i) Determination of antimony (III) and arsenic (III) (by direct Method)
ii) Determination of aluminium, cobalt and zinc (by oxine method)

(c) **EDTA titrations**
i) Determination of copper, nickel, magnesium
ii) Back titration
iii) Alkalimetric titration
iv) Titration of mixtures using masking and demasking agents
v) Determination of hardness of water

2. **Commercial Analysis:**

i) Determination of available chlorine in bleaching powder
ii) Determination of oxygen in hydrogen peroxide.
iii) Determination of phosphoric acid in commercial phosphoric acid.
iv) Determination of boric acid in borax.
v) Determination of metals: copper in copper oxychloride and zinc in zinebfungicides.

3. Analysis of mixtures by gravimetric and volumetric methods from the mixture solutions:

1. Copper- Nickel
2. Copper-Magnesium
3. Copper-Zinc

4. Iron-Magnesium
5. Silver-Zinc
6. Copper-Nickel-Zinc
7. Fe(II)-Fe(III)

4. Green methods of Preparation of the following:

1. Bis(acetylacetonato)copper(II)
2. Tris(acetylacetonato)iron(III)
3. Tris(acetylacetonato)manganese(III)

Books recommended:

1. *A text Book of Quantitative Inorganic Analysis: A.I.Vogl.*
2. *Applied Analytical Chemistry: Vermani.*
3. *Commercial Methods of Analysis: Shell & Biffen*

SEMESTER-I

L	T	P	Credit
0	0	2	2

CHEM-CC-417P: Organic Chemistry Practical-I

Course Objectives	The objectives of present practical course is to trained the students to learn various practical techniques for synthesis, identification, isolation, purification and characterization of organic compounds; and to carry out hand on experience the various methods of organic synthesis**.**
Course Outcomes	At the end of the course, the students will be able to • Apply various methods techniques in organic synthesis to build organic molecules. • Understand the fundamental mechanistic pathways of organic synthesis involving various practical lab techniques together. • Apply the spectroscopic techniques for the determination of molecular structures of organic molecules. • Present their work with practical skills and the awareness of health and safety procedures.

DETAILED CONTENT

Qualitative Analysis:

I. Separation, purification and identification of binary mixture of organic compounds by chemical tests,
II. Thin Layer Chromatography
III. Column Chromatography
IV. IR spectroscopy.

Organic Synthesis:

A. Acetylation: - Acetylation of cholesterol and separation of cholesteryl acetate by column chromatography.
B. Oxidation: Adipic acid by chromic acid oxidation of cyclohexanol.
C. Grignard reaction: Synthesis of triphenyl methanol from benzoic acid.
D. Aldol condensation: Dibenzal acetone from benzaldehyde.
E. Sandmeyer reaction: p-chlorotoluene from p-toluidine.
F. Acetoacetic ester condensation: Synthesis of ethyl-n-butylacetoacetate by A.E.E condensation.
G. Preparation of iodoform from acetone (Haloform reaction).
H. Preparation of polystyrene, anthranilic acid, fluorosceine-eosin, and methyl orange.

Books recommended:

1. Experiments and Techniques in Organic Chemistry, D.Pasto, C. Johnson and M.Miller, Prentice Hall.

2. Macroscale and Microscale Organic Experiments, K.L. Williamson, D.C.Heath.

3. Systematic Qualitative Organic Analysis, H.Middleton, Adward Arnold.

4. Handbook of Organic Analysis-Qualitative and Quantitative, H.Clark, Adward Arnold. 5. Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley.

SEMESTER-I

L	T	P	Credit
0	0	2	2

CHEM-CC-418P: Physical Chemistry Practical-I

Course Objectives	The objective of this course is to have hand-on experiences of techniques for verifying physical and chemical properties and to provide students practical knowledge and skills about various topics taught in theory class of physical chemistry.
Course Outcomes	After the completion of the course, the students should be able to • Understand the basic procedures for carrying out a physical chemistry practical like preparation and standardization of solutions, handling the equipment's and measuring with precision. • Develop experimental skills on conductivity meter, refractometer and stalagmometer for different applications and to interpret the experimental results. • Verify various laws studied in the theory part.

DETAILED CONTENT

1. **Refractive Index (RI) Measurements**: Refractive index (RI) measurements of pure solvents, analysis of mixtures of two miscible solvents, molar and atomic refraction determination, polarizability of liquids.

2. **Conductometric Measurements**: Determination of cell constant, limiting molar conductance of simple electrolytes in water, verification of Ostwald dilution law for week acetic acid.

3. **Surface Tension Measurements**: Surface tension of pure solvents, analysis of mixtures of two miscible solvents, verification of Gibb's Thomson Rule of surface tension.

4. **Partition - Coefficient**: Determination of partition - coefficient for I_2 between water and CCl_4 and for benzoic acid between water and benzene.

5. **Adsorption Measurements**: Verification of Freundlich adsorption isotherm for I_2, acetic acid and oxalic acid on charcoal.

6. **Colloidal Solution**: Preparation of sol solution of arsenic sulphide and estimation of flocculation value for NaCl, KCl, $BaCl_2$, $AlCl_3$.

7. Thermochemistry: Determination of water equivalent of thermos flask, and estimation of heat of neutralization for strong acid strong base, weak acid strong base or vice -versa, heat of hydration and solution of salts.

8. **Kinetic Measurement**: Kinetics of hydrolysis of methyl acetate and ethyl acetate in the presence of HCl.

Books recommended:

1. Senior Practical Physical Chemistry: B.D. Khosla, V.C. Garg and A. Khosla

2. *Experimental Physical Chemistry: V. Athawale and P. Mathur.*
3. *Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.*
4. *Practical in Physical Chemistry: P.S. Sindhu*

SEMESTER-II

Inorganic Chemistry-II

L	T	P	Credit
4	0	0	4

CHEM-CC-421: Metal Ligand Bonding & Magnatochemistry

Course Objectives	The objective of this course is to teach the fundamental and advanced concepts of, electronic spectra charge transfer spectra and magnetic properties of metal complexes.
Course Outcomes	Students are able to : • Interpret electronic and magnetic properties of coordination compounds. • Derive spectroscopic terms for various electronic configurations and their correlation diagrams. • Explain the bonding in complexes using molecular orbital theory.

DETAILED CONTENT

MODULE-I

Metal-Ligand Bonding-I: Recapitulation of crystal field theory including splitting of d-orbitals in different environments, factors affecting the magnitude of crystal field splitting, structural effects (ionic radii, Jahn-Teller effect), thermodynamic effects of crystal field theory (ligation, hydration and lattice energy), limitations of crystal field theory, adjusted crystal field theory (ACFT), evidences for metal-ligand overlap in complexes, molecular orbital theory for octahedral, tetrahedral and square planar complexes (excluding mathematical treatment)

MODULE-II

Atomic Spectroscopy: Energy levels in an atom, coupling of orbital angular momenta, coupling of spin angular momenta, spin orbit coupling, spin orbit coupling p^2 case, determining the ground state terms-Hund's rule, hole formulation (derivation of the term symbol for a closed sub-shell, derivation of the terms for a d^2 configuration), calculation of the number of the microstates.

MODULE-III

Electronic Spectra-I: Splitting of spectroscopic terms (S,P,D,F and G,H,I), d^1-d^9 systems in weak fields (excluding mathematics), strong field configurations, transitions from weak to strong crystal fields.

Electronic Spectra-II: Correlation diagrams (d^1-d^9) in O_h and T_d environments spin-cross over in coordination compounds. Tanabe Sugano diagrams, Orgel diagrams, evaluation of B, C and β parameters.

MODULE-IV

Electronic Spectra - III (Electronic spectra of complex ions): Selection rules (Laporte, orbital and spin selection rules), band intensities, band widths, spectra in solids, spectra of aqueous solutions of d^1-d^9 ions in O_h and T_d environments, evaluation of 10 D_q, spectrochemical and nephelauxetic series, charge- transfer spectra.

MODULE-V

Magnetochemistry: Origin of magnetic moment, factors determining paramagnetism, application of magnetochemistry in co-ordination chemistry (spin only moment, Russell Saunders coupling, quenching of orbital angular moment, orbital contribution to a magnetic moment) in spin free and spin paired octahedral and tetrahedral complexes. Magnetic susceptibility(diamagnetic, paramagnetic), magnetic moments from magnetic susceptibilities, Van Vlecks formula for magnetic susceptibility, temperature dependence of magnetic susceptibility.

Books recommended:

1 Advanced Inorganic Chemistry - Cotton and Wilkinson

2 Coordination Chemistry- Experimental Methods - K.Burger

3 Theoretical Inorganic Chemistry - Day and Selbin

4 Magnetochemistry - R.L.Carlin

5 Comprehensive Coordination Chemistry - Wilkinson, Gillars and McCleverty.

6 Inorganic Electronic Spectroscopy - A.B.P.Lever

7 Concise Inorganic Chemistry - J.D.Lee

8 Introduction to Ligand Fields - B.N.Figgis

9 Physical Methods in Inorganic Chemistry-R.S.Drago

10 Introduction to Magnetochemistry - A.Earnshaw, Academic Press.

SEMESTER-II

L	T	P	Credit
4	0	0	4

CHEM-CC-422: Aromatic, Elimination and Pericyclic Reactions

Course Objectives	The objective of present course is to enrich the students with comprehensive knowledge of the principles of pericyclic reactions and their current applications; fundamental and advanced concepts in reaction mechanisms in organic chemistry along with the reaction mechanisms in various types of aromatic substitution and elimination reactions; to predict and account for the most commonly encountered naming reactions and their mechanisms in organic chemistry; and to use different organic reagent in synthesis. This course will give an emphasis on importance of various reagents in organic synthesis.
Course Outcomes	At the end of the course, the student will be able to • Predict the concerted mechanism of the pericyclic reactions without the involvement of an intermediate. • Predict the thermal or photochemical feasibility of the pericyclic reactions along with their stereo-specificity. • Predict the products of various aromatic nucleophilic and electrophilic substitution reactions. • To predict the role of various reagents in organic synthesis.

DETAILED CONTENT

MODULE - I

(A) **Aromatic Electrophilic Substitution**: Arenium ion mechanism, orientation and reactivity, energy profile diagrams, the ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles, diazonium coupling, Vilsmeir reaction, Scholl reaction, amination reaction, Fries rearrangement, reversal of Friedel Craft alkylation, decarboxylation of aromatic acids.

(B) **Aromatic Nucleophilic Substitution**: SNAr, SN^1, benzyne and SRN^1 mechanism. Reactivity, effect of substrate structure, leaving group and attacking nucleophile, Von Richter, Sommelet-Hauser, and Smiles rearrangements, Ullman reaction, Ziegler alkylation, Schiemann reaction.

MODULE-II

Common Organic Reactions and Their Mechanisms: Perkin condensation, Michael reaction, Robinson annulation, Diekmann reaction, Stobbe condensation, Mannich reaction, Knoevenagel condensation, benzoin condensation, Witting reaction, hydroboration, hydrocarboxylation, ester hydrolysis, epoxidation.

MODULE- III

Reagents in Organic Synthesis: Synthesis and applications of BF_3, NBS, diazomethane, lead tetra-acetate, osmium tetraoxide, Woodward Prevorst hydroxylation reagent, $LiAlH_4$, Grignard reagent, organozinc and

organolithium reagent.

MODULE-IV

Elimination Reactions: Discussion of E_1, E_2, E_1cB and E_2C mechanisms and orientation, reactivity: Effects of substrate structures, attacking base, leaving group and medium. Cis elimination, elimination in cyclic systems, eclipsing effects, pyrolytic eliminations, cleavage of quaternary ammonium hydroxides, fragmentations: γ-Amino and γ-hydroxy halides, decarboxylation of β-hydroxy carboxlic acid and β-lactones.

MODULE-V

Pericyclic Reaction: Molecular orbital symmetry, frontier orbitals of ethylene, 1,3-butadiene, 1,3,5 hexatrienes and allyl system. Classification of pericyclic reactions, Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions: conrotatory and disrotatory motions, 4n and 4n+2 and allyl systems. Cycloadditions- antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and chelotropic reactions. Sigmatropic rearrangements-Suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, Claisen, Cope and aza-Cope rearrangements, Ene reaction.

Books recommended:

1. *Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.*
2. *Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Plenum.*
3. *A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.*
4. *Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University Press.*
5. *Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice Hall.*
6. *Modern Organic Reactions, H.O. House, Benjamin.*
7. *Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic and Professional.*
8. *Pericyclic Reactions, S.M. Mukherji, Macmillan, India.*
9. *Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan.*
10. *Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.*

SEMESTER-II

L	T	P	Credit
4	0	0	4

CHEM-CC-423: Thermodynamics & Electrochemistry

Course Objectives	The main objective of the course is to impart knowledge of classical thermodynamics and electrochemistry, and to provide the understanding of basic concepts of different laws of thermodynamics, chemical equilibria and phase equilibria.
Course Outcomes	After the completion of this course, the students should be able to • Explain the spontaneity of a process and the conditions required for a spontaneous process. • Define a thermodynamical state and differentiate state variable and function. • Calculate the entropy and internal energy of reactants from spectroscopic parameters. • Understand the definition and application of chemical potentials. • Derive and apply Maxwell's relations, the Gibbs-Duhem and Gibbs Helmholtz laws. • Understand Clausius Clapeyron equation and its applications and assess colligative effects. • Understand the concept of phase and derivation of phase rule. Study the phase diagram for one component, two completely miscible component and eutectic systems. • Understand the Debye Huckel Theory of ion-ion interactions and idea of ion-solvent interactions and ion-ion interactions.

DETAILED CONTENT

MODULE – I

Brief resume of law of thermodynamics. Gibb's and Helmholtz free energy functions and their significance. Partial molar quantities. Partial molar free energy and its variation with temperature and pressure. Determination of partial molar volume. Thermodynamic criteria for the feasibility of the process in terms of entropy change, internal energy change, enthalpy and free energy (Gibb's and Helmholtz) change. Gibb's and Helmholtz equation and its utility in thermodynamics of cell reaction. Maxwell's relations. Joule-Thomson effect.

MODULE – II

Chemical potential in case of ideal gases. Thermodynamics of ideal solutions. Fugacity and activity and their variation with temperature and pressure. Graphical method for the determination of fugacity. Chemical equilibrium constant and its temperature dependence. Law of chemical equilibrium and its application.

MODULE – III

Clausius and Clapeyron equation and its application for the determination of colligative properties (depression in freezing point, elevation in boiling point and relative lowering of vapour pressure). Determination of molecular weight of non – volatile solutes from colligative properties. Relationship between relative lowering of vapour pressure and osmotic pressure. Van't Hoff equation for dilute solutions and its application.

MODULE – IV

Nernst heat theorem and third law of thermodynamics and its application. Phase rule and its thermodynamic derivation. Application of phase rule in one and two component systems. Distribution law, its thermodynamic derivation and applications. Zeroth law of thermodynamics.

MODULE –V

Electrochemical equilibrium, Nernst equation, ionic conduction: non – ideal behaviour of electrolytic solutions. Electrolytical potential. Derivation of Debye – Huckel limiting law, extended Debye – Huckel law. Structure of solutions. Detailed treatment of ion – solvent interactions (ion solvation), solvation number. Ion – ion interactions (ion – association). Bjerrum's theory of ion – association.

Books Recommended:

1. Thermodynamics for Chemists: S. Glasstone
2. Physical Chemistry: G.M. Barrow
3. Non – equilibrium Thermodynamics: C. Kalidas
4. Non – equilibrium Thermodynamics: I. Prigogene
5. Electrochemistry: S. Glasstone
6. Electrochemistry: P.H. Reiger
7. Thermodynamics; R.C. Srivastava, S.K. Saha and A.K. Jain
8. Modern Electrochemistry Vol. I: J.O'M Bockris and A.K.N. Reddy

SEMESTER-II

L	T	P	Credit
4	0	0	4

CHEM-CC-424: Organic Spectroscopy and Photochemistry

Course Objectives	The objective of present course is to make the students familiar with various techniques of spectrometric identification of organic compounds; to characterize organic compounds by applying various techniques together; and to provide the comprehensive knowledge of principles of photochemistry reactions with learning of current applications.
Course Outcomes	At the end of the course, the student will be able to • Solve structural problems based on UV-Vis, IR, 1H-NMR, 13C-NMR and mass spectral data. • Elucidate the structures of various organic compounds on the basis of spectral data. • Understand various involved processes responsible for NMR chemical shifts and splitting patterns and mass spectrometry. • Illustrate the mechanisms that give rise to the infrared and UV-Visible absorption bands and identify to which functional groups each correspond. • Understand the basics of photochemical reactions of alkenes, carbonyl and aromatic compounds. • Understand the role of light in the organic synthetic methods and techniques for the applications in chemical reactions

DETAILED CONTENT

MODULE-I

Spectroscopy:

Ultra Violet and Visible Spectroscopy: Electronic transitions (185-800 nm), Beer- Lambert law, effect of solvent on electronic transitions, Ultra Violet bands of carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes. Fieser-Woodward rules for conjugated dienes and carbonyl compounds, Ultra-Violet spectra of aromatic and heterocyclic compounds. Steric effect in biphenyls. Applications of UV- visible spectroscopy in organic chemistry.

Infrared Spectroscopy: Instrumentation and sample handling, characteristic vibrational frequencies of common organic compounds. Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance. Introduction to Raman spectroscopy. Applications of IR and Raman spectroscopy in organic chemistry.

MODULE-II

Nuclear Magnetic Resonance (NMR) Spectroscopy: General introduction, chemical shift, spin-spin interaction, shielding mechanism, chemical shift values and correlation of protons present in different groups in organic compounds. chemical exchange, effect of deuteration, complex spin-spin interaction between two, three, four and five nuclei, virtual coupling. Stereochemistry, hindered rotation, Karplus-relationship of coupling constant with dihedral angle. Simplification of complex spectra-nuclear magnetic double

resonance, spin tickling, INDOR, contact shift reagents, solvent effects. Fourier transform technique, Nuclear Overhauser Effect (NOE). Introduction to resonance of other nuclei -F, P, principle and introduction to C^{13} NMR, 2-D and 3-D NMR, applications of NMR in organic chemistry.

MODULE-III

Mass Spectrometry: Introduction, ion production—EI, CI, FD and FAB, factors affecting fragmentation, ion analysis, and ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, Molecular ion peak, Meta-stable peak, McLafferty rearrangement. Nitrogen rule. High-resolution mass spectrometry. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination. Introduction to negative ion mass spectrometry, TOF-MALDI. Problems based upon IR, UV, NMR and mass spectroscopy.

MODULE- IV

Photochemistry - I: Introduction and basic principles of photochemistry. Interaction of electromagnetic radiations with matter. Types of excitations, fate of excited molecules, quantum yield, transfer of excitation energy, actinometry. Photochemistry of alkenes: cis-trans isomerization, dimerization of alkenes, photochemistry of conjugated olefins, photo-oxidation of alkenes and polyenes photochemistry of aromatic compounds: Isomerization, addition and substitution, photo-reduction of aromatic hydrocarbons.

MODULE- V

Photochemistry - II: Photochemistry of carbonyl compounds: Norrish type I and II, intermolecular and intramolecular hydrogen abstraction, Paterno-Buchi reaction, α and β- cleavage reactions of cyclic and acyclic carbonyl compounds, formation of oxetane and cyclobutane from α, β unsaturated ketones, photo-reduction of carbonyl compounds, photo-rearrangement of enones, dienones, epoxyketones, Photo Fries rearrangement.

Books recommended:

1. *Practical NMR Spectroscopy, M.L. Martin, J.J. Delpeuch and G.J.Martin, Heyden*
2. *Spectrometric Identification of Organic Compounds, R. M. Silverstein, G.C.Bassler and T.C.Morrill, John Wiley.*
3. *Introduction to NMR Spectroscopy, R.J. Abraham, J. Fisher and P. Loftus, Wiley.*
4. *Application of Spectroscopy of Organic Compounds, J.R. Dyer, Prentice Hall.*
5. *Spectroscopic Methods in Organic Chemistry, D.H. Williams,I. Fleming, Tata McGraw-Hill.*
6. *Organic spectroscopy by Jagmohan*
7. *Organic spectroscopy by W. Kemp.*
8. *Fundamentals of Photochemistry, K.K.Rohtagi - Mukherji, Wiley-Eastern.*
9. *Essentials of Molecular Photochemistry, A. Gilbert and J.Baggot, Blackwell Scientific Publication.*
10. *Molecular Photochemistry, N.J. Turro, W.A. Benjamin.*
11. *Introductory Photochemistry, A. Cox and T. Camp, McGraw-Hill.*
12. *Photochemistry, R.P. Kundall and A. Gilbert, Thomson Nelson.*
13. *Organic Photochemistry, J. Coxon and B. Halton, Cambridge University Press.*
14. *Organic Photochemistry Vol.I, II, III. Ed. Orville L. Chapman.*
15. *Organic Photochemistry, Ed. Robert O. Kan.*

SEMESTER-II

L	T	P	Credit
0	0	2	2

CHEM-CC-425P: Inorganic Chemistry Practical-II

Course Objectives	It deals with qualitative and quantitative inorganic analysis along with preparation of inorganic complexes.
Course Outcomes	Students are able to: • Apply these ideas in various fields pertaining to inorganic chemistry. • Apply their knowledge on accuracy, precession and error of readings. • Communicate the results of the experiment in a written and oral form.

DETAILED CONTENT

Preparation of the following compounds and a study of the important properties viz. Molar conductance, magnetic sussceptibility, electronic and infrared spectra.

1. Stannic iodide
2. Bis(acetylacetonate) oxovanadium (IV)
3. Tris (acetylacetonate) siliconchloride.
4. Mercuration of phenol.
5. Hexa ammine nickel (II) chloride.
6. Pyridine perchromate.

INSTRUMENTAL ANALYSIS:

(A) **Conductometric Titrations**:

i) Differential behaviour of acetic acid to determine the relative acid strength of various acids and basic strength of various bases.

ii) Strong acid-strong base titration in acetic acid.

(B) **Potentiometric Titrations**.

1. Neutralisation reactions:
   - i) Sodium hydroxide-hydrolchloric acid.
   - ii) Sodium hydroxide-Boric acid
   - iii) Acetic acid and hydrochloric acid-sodium hydroxide.
2. Oxidation-Reduction Reactions.
   - i) Ferrous-dichromate
   - ii) Ferrous-Ceric
   - iii) Iodine-Thiosulphate
3. Precipitation Reactions:

i) Silver nitrate-sodium halides.

4. Complexation Reactions
   i) Potassium cyanide-silver nitrate.

(C) **Colorimetric Analysis**:

1. Verification of Beer's law for $KMNO_4$, $K_2Cr_2O_7$ solutions and determination of the conc. of $KMNO_4$ $K_2Cr_2O_7$ in the given solution.
2. Colorimetric determination of Iron (III) with potassium thiocyanate reagent or o-Phenanthroline method.
3. Determination of traces of manganese (in steel samples) colorometrically byoxidation to permanganic acid with potassium periodate.
4. Spectrophotometric determination of pK value of an indicator (acid dissociation constt. of methyl red)

(D) **pH metric –titrations**

1. Copper and cactechol
2. Copper and salicylic acid
3. Acid base titrations
4. Mixtures of acids with a base

(E) **Polarography:**

1. Determination of half wave potentials of cadmium ion in potassium chloride solution
2. Determination of half wave potentials of zinc and manganous ions in potassium
3. Determination of cadmium in solution
4. Investigation of the influence of dissolved oxygen.

(F) **Amperometric Titrations:**

1. Zinc with EDTA
2. Lead vs. chromate
3. Nickel as isoquilnoline thiocynate

(G) **Flame Photometry:**

1) Determination of sodium
2) Determination of potassium
3) Determination of calcium

(H) **Miscellaneous:**

1. Determination of stability constants of complexes.
2. Determination of magnetic susceptibility of complexes
3. Estimation of periodate, iodate and bromate in the same solution.
4. Determination of bromide and chloride in the same solution.
5. Analysis of a solution containing chloride and iodide.

Books recommended:

1. *A Text Book of Quantitative Inorganic Analysis- A.I. Vogel*
2. *Chemistry Experiments for Instrumental Methods:- D.T. Sawyer, W.R. Heinemanand J.M. Beebe.*
3. *Inorganic Synthesis- R.A. Rowe and M.M. Jones (1957)5, 113 - 116.*

SEMESTER-II

L	T	P	Credit
0	0	2	2

CHEM-CC-426P: Organic Chemistry Practical-II

Course Objectives	To provide the students practical experience in techniques used in the synthesis, isolation, characterization and structure determination of organic compounds.
Course Outcomes	At the end of the course, the student will be able to • Interpret the compounds using UV-Vis, FT-IR, PMR, CMR and MS techniques. • Extract and separate different organic compounds using chromatography techniques • Apply related experiments for their research work.

DETAILED CONTENT

(A) **Extraction of Organic Compounds from Natural Sources**: Isolation of caffeine from tea leaves, casein from milk (the students are required to try some typical colour reactions of proteins), lactose from milk (purity of sugar should be checked by TLC and PC and Rf value reported). Lycopene from tomatoes and β- carotene from carrots.

(B) **Paper Chromatography**: Separation and identification of the sugars present in the given mixture of glucose, fructose and sucrose by paper chromatography and determination of Rf values.

(C) **Spectroscopy**:

Identification of some organic compounds by the analysis of their spectral data (UV, IR, PMR, CMR and MS)

- Multistep
- Synthesis of Vacor
- Synthesis of Indigo
- Synthesis of p- nitro aniline

Books recommended:

1. *Experiments and Techniques in Organic Chemistry, D.Pasto, C. Johnson and M.Miller, Prentice Hall.*
2. *Macroscale and Microscale Organic Experiments, K.L. Williamson, D.C.Heath.*
3. *Systematic Qualitative Organic Analysis, H.Middleton, Adward Arnold.*
4. *Handbook of Organic Analysis-Qualitative and Quantitative, H.Clark, Adward Arnold.*
5. *Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley.*

SEMESTER-II

L	T	P	Credit
0	0	2	2

CHEM-CC-427P: Physical Chemistry Practical-II

Course Objectives	To impart training in operating different instruments used in the analysis of various chemical constituents and to provide students practical knowledge about basic techniques.
Course Outcomes	Student will be able to • Design and develop experimental skills on experiments in Physical Chemistry using potentiometry, conductometry, colorimetry, viscometry, kinetics and polarimetry. • Apply concepts of Physical Chemistry through experimentation. • To describe the principles behind the experiment performed in the laboratory.

DETAILED CONTENT

1. **Viscosity Measurements**: Verification of the Jones - Dole equation, determination of viscosity A and B - coefficients for simple electrolytes in water and in aqueous mixtures of organic solvents.

2. **Conductometric Measurements**: Kinetics of saponification of ethyl acetate by NaOH. Solubility of sparingly soluble salts.

3. **Potentiometric Titration**: Titration of HCl with NaOH, determination of dissociation constant of acetic acid and phosphoric acid. Oxidation - reduction titration (ferrous ammonium sulphate with $KMnO_4$ and $K_2Cr_2O_7$).

4. **Flame photometric Measurements**: Establishing the calibration plots for Na^+ and K^+ ions and determination of their concentration in the given solution at ppm level.

5. **Determination of Molar Mass**: Cryoscopic and Rasts's methods. Determination of molar mass of polymer by viscosity measurement.

6. **Colorimeter Measurements**: Determination of composition ferric ions – salicylic acid complex using Job's method.

7. **Polarimetry Measurements**: Determination of specific and molecular rotation, percentage of two optically active substances, kinetics of acid catalysed inversion of cane sugar, comparison of strengths of two acids.

Books recommended:

1. *Senior Practical Physical Chemistry: B.D. Khosla, V.C. Garg and A. Khosla*
2. *Experimental Physical Chemistry: V. Athawale and P. Mathur.*
3. *Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.*
4. *Practical in Physical Chemistry: P.S. Sindhu*
5. *Senior Practical Physical Chemistry: B.D. Khosla, V.C. Garg and A. Khosla*

SEMESTER-III

L	T	P	Credit
4	0	0	4

CHEM-CC-431: Analytical & Nuclear chemistry

Course Objectives	The objective of this course is to develop interest and understanding about the basic concepts of the subject. Nuclear reaction and radioactivity, chemical periodicity and physical properties of F-block elements.
Course Outcomes	Students are able to: • Use the basic statistical treatment of the analytical data for getting a correct result. • Able to illustrate different type's nuclear models and their features. • Apply their knowledge on accuracy, precession and error of readings.

DETAILED CONTENT

MODULE-I

Metal π Complexes: Preparation, reactions, structures and bonding in carbonyl, nitrosyl, phosphine and related complexes, structural evidences from vibrational spectra, bonding and important reactions of metal carbonyls. Structure and bonding in metal cyanides, stabilization of unusual oxidation states of transition metals.

MODULE-II

Introductory Analytical Chemistry: Data analysis- types and sources of errors, propagation of errors, detection and minimization of various types of errors. Accuracy and precision, average and standard deviation, variance, its analysis and confidence interval, tests of significance (F-test, t-test and paired t-test), criteria for the rejection of analytical data (4d rule, 2.5d rule, Q-test, average deviation and standard deviation), least-square analysis.

Food and Drug Analysis- General methods for proximate and mineral analysis in food (moisture, ash, crude fiber, nitrogen (proteins) and minerals (iron, calcium, potassium, sodium and phosphorus). Discussion of official (pharmacopeia) methods for the determination of following drugs as such: (i) Analgin/oxyphenbutazone, (ii) chloramphenicol and related nitro compounds, (iii) chloroquinine, (iv) phenyl butazone, (v) salicylic acid and (vi) sulphonamides.

MODULE-III

Photoelectron Spectroscopy: Basic principle, photoionization process, ionization energies, Koopman's theorem, ESCA, photoelectron spectra of simple molecules, (N_2, O_2 and F_2). Photoelectron spectra for the isoelectronic sequence Ne, HF, H_2O, NH_3 and CH_4, chemical information from ESCA, Auger electron spectroscopy - basic idea.

MODULE-IV

Lanthanides and Actinides:- Spectral and magnetic properties, comparison of inner transition and transition metals, transuranium elements (formation and colour of ions in aqueous solution),uses of lanthanide compounds as shift reagents, periodicity of translawrencium elements.

MODULE-V

Nuclear Chemistry: Nuclear binding energy and stability, nuclear models (nuclear shell model and collective model). Nuclear reactions: types of reactions, nuclear cross-sections, Q-value. Natural and artificial radioactivity, radioactive decay and equilibrium, nuclear fission-fission product and fission yields, nuclear fusion.

Radioactive techniques: Tracer technique, (neutron activation analysis), Counting techniques such as G.M. ionization and proportional counters.

Books recommended:

1. *Advanced Inorganic Chemistry - Cotton and Wilkinson*
2. *Fundamentals of Analytical Chemistry - Skoog and West*
3. *Quantitative Inorganic Analysis - Vogel*
4. *Chemistry of the Elements - Greenwood and Earnshaw*
5. *Nuclear Chemistry-U.C.Dash*
6. *Nuclear Chemistry - B.G.Harvey*
7. *Nuclear Chemistry - Arnikar*
8. *Techniques in Inorganic Chemistry Vol. II (Nuclear Chemistry-Johnson and Others).*
9. *Modern Aspects of Inorganic Chemistry-H.J.Emeleus and A.G.Sharpe*
10. *Inorganic Chemistry, 4th Edition, - J.E.Huheey, E.A.Keiter and R.L.Keiter.*
11. *Analytical Chemistry-G.D.Christian*
12. *Chemical Structure and Bonding- Dekock and Gray*
13. *The Organometallic Chemistry of Transition metals: R.H. Crabtree.*
14. *Electronic absorption spectroscopy and related techniques: D.N. Sathyanarayan*

SEMESTER-III

L	T	P	Credit
4	0	0	4

CHEM-CC-432: Statistical Thermodynamics and Basic Quantum Chemistry

Course Objectives	This course will equip students with the necessary chemical changes based on the foundation of thermodynamics, partition function thermodynamic system of vibration, free energy, electromotive force, standard entropy etc. Also, it helps students to use statistical physical system as models to understand complex system. To impart students' knowledge regarding basics of Quantum mechanics and their applications for solving various problems in physical chemistry.
Course Outcomes	At the end of the course, the student will be able to • Understand the need for quantum mechanical formalism and basic principles. • Appreciate the importance and implication of generalized uncertainty principle in quantum mechanics. • Apply Schrodinger wave equation and approximation methods for problem solving in quantum mechanics. • Solve various problems related to non-ideal systems. • Define the dynamics of various types of reactions. • Rationalize bulk properties and processes using thermodynamic considerations.

DETAILED CONTENT

Statistical Thermodynamics

MODULE – I

Basic Terminology, probability, phase space, micro and macro states, thermodynamic probability, statistical weight, assembly, ensemble and its types. The most probable distribution: Maxwell-Boltzmann distribution, Quantum statistics: The Bose- Einstein statistics and Fermi- Dirac statistics. Thermodynamic probability (W) for the three types of statistics. Lagrange's undetermined multipliers, Stirling's approximation. Molecular partition function for an ideal gas. Evaluation of translational, rotational, vibrational, nuclear and electronic partition function.

MODULE – II

Rotational partition function of homonuclear diatomic molecules. Thermodynamic properties of molecules from partition function: Total energy, entropy, Helmholtz free energy, pressure, heat content, heat capacity and Gibb's free energy. Relation between equilibrium constant and partition function. Heat capacity of crystals and statistical thermodynamics.

Basic Quantum Chemistry

MODULE – III

Operators in quantum mechanics. Eigenvalues and eigenfunctions. Hermitian operator and its application. Postulates of quantum mechanics. Angular momentum of a one – particle system and its commutative relations. Schrodinger wave equation and its formulation as an eigenvalue problem. The uncertainty principle.

MODULE – IV

Quantum mechanical treatment of translational motion of a particle, particle in one and three dimensional boxes, harmonic – oscillator, Rotational motion of a particle: particle on a ring, particle on a sphere, rigid rotator and hydrogen atom. Graphical presentation of orbitals (s, p and d), radial and angular probability distribution plots.

Photochemistry

MODULE – V

Photophysical processes of electronically excited molecules (Jablonski diagram). Frank – Condon principle: a quantum – mechanical treatment. Energy transfer from electronically excited molecules: Stern – Volmer equation. Photophysical pathways: fluorescence, phosphorescence, E-type and P- type delayed fluorescence. Kinetic treatment of excimer and exciplex formation.

Books Recommended:

1. Physical Chemistry: D.W. Ball
2. Theoretical Chemistry by S. Glasston
3. Statistical Chemistry by I. Prigogine
4. Quantum Chemistry An Introduction: H.L. Strauss
5. Introductory Quantum Chemistry: A.K. Chandra
6. Quantum Chemistry: A. Mcquarrie
7. Quantum Chemistry: I.N. Levine

SEMESTER-III

L	T	P	Credit
4	0	0	4

RM-CC-022: Research Methodology

Course Objectives	This course will help to: Develops better insight into topic; Provides systematic structure; Enhance the research quality; Derive better solutions; Aids in decision making; Inculcates logical and systematic thinking.
Course Outcomes	At the end of this course, the students should be able to: • understand some basic concepts of research and its methodologies • identify appropriate research topics • select and define appropriate research problem and parameters • prepare a project proposal (to undertake a project) • organize and conduct research (advanced project) in a more appropriate manner • write a research report and thesis • write a research proposal (grants)

DETAILED CONTENT

MODULE-I

Foundations of Research: Meaning, objectives, motivation, utility. Concept of theory, empiricism, deductive and inductive theory. Characteristics of scientific method – Understanding the language of research – Concept, construct, definition, variable, research process.

Problem Identification & Formulation – Research question – investigation question –measurement issues – Hypothesis – qualities of a good hypothesis –null hypothesis & alternative hypothesis. Hypothesis testing – logic & importance.

MODULE-II

Research Design: Concept and importance in Research – Features of a good research design. Exploratory research design – concept, types and uses, Descriptive research designs – concept, types and uses. Experimental Design: concept of independent & dependent variables.

Qualitative and Quantitative Research: Qualitative research – Quantitative research – Concept of measurement, causality, generalization, replication. Merging the two approaches.

MODULE-III

Measurement: Concept of measurement– what is measured? Problems in measurement in research – validity and reliability. Levels of measurement – Nominal, Ordinal, Interval, Ratio.

Sampling: Concepts of statistical population, sample, sampling frame, sampling error, sample size, non-response. Characteristics of a good sample. Probability Sample – simple random sample, systematic sample,

stratified random sample & multi-stage sampling. Determining size of the sample – practical considerations in sampling and sample size.

MODULE-IV

Data Analysis: Data preparation – Univariate analysis (frequency tables, bar charts, pie charts, percentages), Bivariate analysis – Cross tabulations and Chi-square test including testing hypothesis of association. **Interpretation of Data and Paper Writing** – Layout of a research paper, Journals in chemical sciences, Impact factor of Journals, when and where to publish? Ethical issues related to publishing, Plagiarism and self-Plagiarism.

MODULE-V

Use of tools / techniques for Research: Methods to search required information effectively, Reference Management Software like Zotero/Mendeley, Software for paper formatting like LaTeX/MS Office, Software for detection of Plagiarism. Use of Encyclopaedias, Research guides, Handbook etc., Academic databases for computer science discipline.

Books recommended:

1. *Business Research Methods – Donald Cooper & Pamela Schindler, TMGH, 9th edition*

2. *Business Research Methods – Alan Bryman & Emma Bell, Oxford University Press.*

3. *Research Methodology – C.R.Kothari*

4. *Select references from the Interne*

SEMESTER-III

L	T	P	Credit
0	0	2	2

CHEM-CC-436P: Inorganic Chemistry Practical-III

Course Objectives	The objective of this course is to provide practical knowledge and illustrative experiments about synthesis and characterization of inorganic complexes.
Course Outcomes	Students are able to: • Design a scheme for synthesis of coordination compound and execute it based on the principles learned. • Solve problems encountered during a synthesis.

DETAILED CONTENT

1. Analysis of the given sample (Ores)/Both Qualitative and Quantitative Dolomite, Pyrolusite, Galena.

2. Analysis of the given alloys: Coin, Gunmetal, Brass and Bronze.

3. To prepare a pure and dry sample of the following compounds:

1. Potassium tris(oxalato)aluminate(III)
2. Sodium hexa(nitro)cobaltate(III)
3. Potassium tris(oxalato)cobaltate(III)
4. Hexa(ammine)cobalt (III)chloride
5. Tetrapyridine copper(II)persulphate
6. Dinitrotetrapyridine nickel(II)
7. Lead tetraacetate
8. Mercury (tetraisothiocyanato)cobaltate(II).

and characterize them by the following techniques:

i) Elemental analysis
ii) Molar conductance values
iii) I.R. Spectral interpretation
iv) Thermal analysis
v) UV-Visible Spectra

Books recommended:

1. *A Text Book of Qualitative Inorganic Analysis - A.I. Vogel*

SEMESTER-III

L	T	P	Credit
0	0	2	2

CHEM-CC-437P: Organic Chemistry Practical-III

Course Objectives	The objectives of this practical course are make students to learn: how to use the methods for the preparation of useful compounds using named reaction; utilize various methods for preparing organic compounds in a multiple step; to determine the percentage/ number of hydroxyl groups, amines and phenols in given compounds; and to check the BOD, COD and DO in given samples.
Course Outcomes	On completion of the course, students should be able to: • Design and carry out experiments, accurately record and analyze the results of such experiments. • Interpret the compounds using multiple physical techniques.

DETAILED CONTENT

A. **Quantitative Analysis:**

Determination of the percentage/ number of hydroxyl groups in an organic compound by acetylation method. Estimation of amines/ phenols using bromate –bromide solution/ acetylation method. Determination of iodine and sponification values of an oil sample. Determination of DO, COD and BOD of water sample.

B. **Multistep Synthesis:**

Cannizzaro reaction: 4-chlorobenzaldehyde as substrate.

Benzilic Acid Rearrangement: Benzaldehyde → Benzoin→ Benzil→ Benzilic acid. **Hofmann bromamide Rearrangement** : Phthalic anhydride → Phthalimide→ Anthranilic acid

Beckmann Rearrangement: Benzene→Benzophenone→BenzophenoneOxime→Benzanilide.

Skraup Synthesis: Preparation of quinoline from aniline.

Synthesis using Phase Transfer Catalysis: Alkylation of diethyl malonate or ethyl acetoacetate and an alkyl halide.

Books recommended:

1. *Experiments and Techniques in Organic Chemistry, D.Pasto, C. Johnson and M.Miller, Prentice Hall.*
2. *Macroscale and Microscale Organic Experiments, K.L. Williamson, D.C.Heath.*
3. *Systematic Qualitative Organic Analysis, H.Middleton, Adward Arnold.*
4. *Handbook of Organic Analysis-Qualitative and Quantitative, H.Clark,Adward Arnold.*
5. *Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley.*

SEMESTER-III

L	T	P	Credit
0	0	2	2

CHEM-CC-438P: Physical Chemistry Practical-III

Course Objectives	To impart practical knowledge of the concepts and laws used in the theory and provide training in handling different instruments used in the analysis of various chemical constituents.
Course Outcomes	Student will be able to • Design various experiments using thermometry, conductometry, colorimetry, and kinetics. • Apply concepts to construct phase diagrams. • To describe the principles behind the experiment performed in the laboratory.

DETAILED CONTENT

1. **Solubility Measurements**: Heat of solution of electrolytes by solubility measurements.

2. **Heat of transfer Measurements**: Heat of transfer for benzoic acid between benzene and water and I_2 between CCl_4 and water.

3. **Conductometric Measurements**: Precipitation titration ($AgNO_3$ - KCl), acid - base neutralization titration, determination of relative strength of acids in the given mixtures, solubility of sparingly soluble salt.

4. **Construction of Phase Diagram**: Phase diagram for liquids, (benzene and methanol) and phase diagram for solids, (benzoic acid and cinnamic acid, benzoic acid and naphthalene and acetamide and salicylic acid).

5. **Colorimetric Measurements**: Verification of Beer - Lambert's law for aqueous solutions of $KMnO_4$, $K_2Cr_2O_7$ and $CuSO_4$ and construction of calibration plot to estimate the unknown concentration.

6. **Kinetic Measurement**: Saponification of ethyl acetate by NaOH solution.

Books recommended:

1. *Senior Practical Physical Chemistry: B.D. Khosla, V.C. Garg and A. Khosla*
2. *Experimental Physical Chemistry: V. Athawale and P. Mathur.*
3. *Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.*
4. *Practical in Physical Chemistry: P.S. Sindhu*

SEMESTER-III

L	T	P	Credit
0	0	2	2

CHEM-CC-500: Seminar

Objectives	The objectives of seminar are to develop the skill of communication in presentation; to demonstrate the utility of various software such as Chem Draw, Origin, MS-Office etc; to identify the topic with the consideration feasibility; and to help students in searching literature on selected research oriented project work.
Outcomes	On completion of this subject, participants should be able to: • Demonstrate capacity to lead and manage change through collaboration with others • Analyse data and synthesize research findings • Report research findings in written and verbal forms

DETAILED CONTENT

Every candidate will have to deliver a seminar of 15-30 minutes duration on a topic related to his/her project work which will be chosen by him / her in consultation with the teacher of the department. The seminar will be delivered before the students and teachers of the department. A three-member committee (one coordinator and two teachers of the department of different branches) duly approved by the departmental council will be constituted to evaluate the seminar. The following factors will be taken into consideration while evaluating the candidate.

(i) Expression

(ii) Presentation

(iii) Depth of the subject matter and answers to the questions.

SEMESTER-IV

L	T	P	Credit
4	0	0	4

CHEM-CC-441: Techniques of Chemical Analysis

Course Objectives	The primary objective of this course is to acquire basic concepts, principles, and techniques of modern analytical chemistry that would empower students with an analytical mind set and the abilities to solve diverse analytical problems in an efficient and quantitative way that conveys the importance of accuracy and precision of the analytical results.
Course Outcomes	On successful completion of this course, students will be able: • To develop an understanding of the range and uses of analytical methods in chemistry. • To establish an appreciation of the role of chemistry in quantitative analysis. • To develop an understanding of the broad role of the chemist in measurement and problem solving for analytical tasks. • To provide an understanding of chemical methods employed for elemental and compound analysis. • To provide experience in some scientific methods employed in analytical chemistry.

DETAILED CONTENT

MODULE-I

Spectrophotometry: i) Introduction, fundamental laws of photometry, the electromagnetic spectrum and spectrochemical methods, UV/Visible instrumentation, absorption spectra, Beer-Lambert's Law, deviation from Beer-Lambert's Beer's law. ii) photometric titrations:- Simultaneous spectrophotometric determination, differential spectrophotometry, titration curves and applications to quantitative analysis. iii) Molecular Fluorescence Spectroscopy:- Theory, relaxation processes, relationship between excitation spectra and florescence spectra, florescencent species, effect of concentration on florescence intensity, instrumentation and application of florescence methods.

MODULE-II

Atomic Spectroscopy: Theory of flame photometer, intensities of spectral lines, selection of optimal working conditions, applications of flame photometry to quantitative analysis. The Theory of Atomic absorption spectroscopy (AAS), origin of atomic spectra, line width effects in atomic absorption, instrumentation and its application. Atomic emission spectroscopy (AES) and the detailed description of the techniques of inductively coupled plasma AES (ICP-AES) and its instrumentation. Chemical and spectral interferences encountered in both techniques and how to overcome them.

MODULE-III

Electroanalytical Methods

Electrogravimetric methods:- i) Current-voltage relationship during electrolysis, operation of a cell at a fixed applied potential, constant current electrolysis, physical properties of electrolytic precipitates, chemical

factors of importance in electrodeposition, anodic deposition. ii) Spontaneous electrogravimetric analysis (internal electrolysis), apparatus and applications. iii) Electrolytic method with and without potential control, apparatus and applications.

Coulometric Methods: i) Controlled potential coulometry, instrumentation and applications. ii) Coulometric titrations, cell for coulometric titrations, applications of coulometric titrations (neutralization, precipitation, and complex formation titrations), comparison of coulometric and volumetric titrations.

MODULE-IV

Polarographic Methods: General introduction: theoretical measurements of classical polarography, polarographic measurements, polarograms, interpretation of polarographic waves, equation for polarographic waves, half-wave potential, effect of complex formation on polarographic waves, dropping mercury electrode (advantages and limitations), current variation with a dropping electrode, polarographic diffusion current, the ilkovic equation, effect of capillary characterization on diffusion current, diffusion coefficient temperature, kinetic and catalytic current, polarograms for mixtures of reactants, anodic waves and mixed anodic and cathodic waves, current maxima and its suppression, residual current, supporting electrolytes, oxygen waves, instrumentation and applications to inorganic and organic analysis.

MODULE-V

Thermogravimetric analysis: Introduction, Factors affecting thermogravimetric curves, instrumentation, applications to inorganic compounds (analysis of binary mixtures i.e. Ca and Mg, TG curves of calcium oxalate, determination of Ca, Sr & Ba ions in the mixture, drying of sodium carbonate, analysis of clays and soils, decomposition of potassium hydrogen phthalate, oxidation of nickel sulphide, determination of titanium content of non-stoichiometric sample of titanium carbide).

Differential thermal analysis: Introduction, factors effecting DTA curves, instrumentation, applications, to inorganic compounds (thermal decomposition of mixtures of lanthanum-cerium and praseodymium oxalate, DTA curves for $CuSO_4.5H_2O$, sulphur, detection of organic contamination in ammonium nitrate, thermal decomposition for different magnesium carbonate samples, determination of uncalcined gypsum in plaster of paris.

Books recommended:

1. *Instrumental methods of analysis.-H.H.Willard, LL.Marritt and J.A.Dean*
2. *Fundamental of analytical Chemistry -D.A.Skoog & D.M.West*
3. *Basic concepts of analytical Chemistry-S.M.Khopkar*
4. *Instrumental Methods of Chemcial Analysis-G.K.Ewring*
5. *Quantitative Inorganic Analysis-A.I.Vogel*
6. *Ion Exchange-AellFerish*
7. *Modern Polarographic Methods in Analytical Chemistry -A.M.Bond*
8. *Thermal Methods of Analysis-W.W. Wandlandt.*
9. *D.A.Skoog, F.J.Holler and T.E.Nieman, Principles of Instrumental analysis, 5th Edition, Saunder's college Pub. 1998.*

SEMESTER-IV

L	T	P	Credit
0	0	8	8

CHEM-CC-501: Research Project

Project Objectives	The objectives of project work will be to enrich the students: to design research oriented project on particular context; to identify the topic with the consideration feasibility; to search literature on selected research oriented project work; to identify/search the advances in current research; to conduct experiment scientifically with safety; to utilize the techniques learn earlier for the synthesis of bioactive molecules with the help of named reactions and rearrangements; to characterize the prepared molecules by physical and spectral analysis like IR, 1H NMR, ^{13}C NMR and Mass Spectroscopy; to prepare a dissertation report with complete follow up of research methodology; to develop the skill of communication in presentation; to demonstrate the utility of various software such as ChemDraw, Origin, MS-Office etc; and to employ/use the techniques used in typing of dissertation such as Foot Note, End Note etc.
Project Outcomes	On completion of this subject, participants should be able to: • Carry out a substantial research-based project • Demonstrate capacity to improve student achievement, engagement and retention • Demonstrate capacity to lead and manage change through collaboration with others • Demonstrate an understanding of the ethical issues associated with practitioner research • Analyse data and synthesize research findings • Report research findings in written and verbal forms • Use research findings to advance education theory and practice.

Every candidate will have to work on minor project on different topic which will be chosen by him / her in consultation with his/her supervisor. Which include literature review, experimental works and discussions regarding their industrial and commercial applications. A three-member committee (one coordinator and two teachers of the department of different branches) duly approved by the departmental council will be constituted to evaluate the project. The following factors will be taken into consideration while evaluating the candidate.

(i) Project Report—40%

(ii) Presentation-----30%

(i) Viva-Voce------30%

1. Discipline Specific Elective Courses

SEMESTER-III

L	T	P	Credit
4	0	0	4

CHEM-EC-433: Bioinorganic Chemistry and Reaction Mechanism

Course Objectives	The course will provide students with a general overview of the many fundamental tasks performed by inorganic elements in living organisms as well as the related methods and theories with particular emphasis on enzymatic conversions and electron transfer. This goes along with the elucidation of model systems and technical applications of both, concepts learned from nature as well as biological systems.
Course Outcomes	By the end of the course students will be able to: • understand how metal ions interact with biological environments and how these interaction influences the properties of metal centres. • apply principles of coordination chemistry to explain how nature tailors properties of metal centres for specific applications. • answer critical questions (asked by fellow students or the instructor) and engage in scientific discussion on bioinorganic chemistry related topics.

DETAILED CONTENT

MODULE-I

Metalloporphyrins: Porphyrins and their salient features, characteristic absorption spectrum of porphyrins, chlorophyll (structure and its role in photosynthesis). Transport of iron in microorganisms (siderophores), types of siderophores (catecholate and hydroxamato siderophores).

Metalloenzymes: Definitions: Apoenzyme, coenzyme, metalloenzyme, structure and functions of carbonic anhydrase A & B, carboxy peptidases.

MODULE-II

Oxygen Carriers:

Natural oxygen carriers: Structure of hemoglobin and myoglobin, Bohr effect, models for cooperative interaction in hemoglobin, oxygen transport in human body (-perutz mechanism), cyanide poisoning and its remedy. Non-heme proteins (hemerythrin &hemocyanin).

Synthetic oxygen carriers: Oxygen molecule and its reduction products, model compounds for oxygen carrier (Vaska's Iridium complex, cobalt complexes with dimethyl glyoxime and schiff base ligands).

MODULE-III

Transport and storage of metals: The transport mechanism, transport of alkali and alkaline earth metals, ionophores, transport by neutral macrocycles and anionic carriers, sodium/potassium pump, transport and storage of iron (transferrin & ferritin).

Inorganic compounds as therapeutic Agent: Introduction chelation therapy, synthetic metal chelates as antimicrobial agents, antiarthritis drugs, antitumor, anticancer drugs (platinum complexes), Lithium and mental health.

MODULE-IV

Supramolecular Chemistry: Introduction, some important concepts, introduction to recognition, information and complementarity, principles of molecular receptor designs, spherical recognition (cryptates of metal cations) tetrahedral recognition by macrotricyclic cryptands, recognition of ammonium ions, recognition of neutral molecules and anionic substrates (anionic coordination)

MODULE-V

Inorganic Reactions and Mechanism: Substitution reactions in octahedral complexes, acid hydrolysis reactions, base hydrolysis and anation reactions, substitution reaction, reactions occurring without rupture of metal-ligand bond. Substitution reactions of square planar complexes. Theories of trans-effect, labile and inert complexes. Mechanism of redox reactions.

Books recommended:

1. *The Inorganic Chemistry of Biological processes - M.N.Hughes.*
2. *Bio Inorganic Chemistry - Robert Wittay*
3. *Advanced Inorganic Chemistry (4th Edn) - Cotton and Wilkinson.*
4. *Topics in current chemistry (Inorganic Biochemistry) vol. 64 (1976) - Davison and Coworkers.*
5. *An Introduction to Biochemcial Reaction Mechanism - James N.Lowe and Lloyalt Ingraham.*
6. *General Biochemistry - Fruton J.S. and Simmonds S.*
7. *Plant Physiology - Robeert N.Devtin.*
8. *Inorganic chemistry - James E. Huheey.*
9. *Supramolecular Chemistry (Concepts and Perspectives) - Jean Marie Lehn(VCH-1995).*
10. *Advanced Inorganic Chemistry- Cotton and Wilkinson*
11. *Inorganic Reaction Mechanism - Edberg*
12. *Inorganic Reaction Mechanism - Basoloavd Pearsor*

SEMESTER-III

L	T	P	Credit
4	0	0	4

CHEM-EC-434: Natural Products

Course Objectives	The aim and objective of this course is to make students understand the chemistry of common natural products. The course will involve the structure, chemistry and metabolic pathways involving the common natural products.
Course Outcomes	At the end of the course, the student will be able • To learn the chemistry and methods to determine structure elucidation of natural products • To study the chemistry of chemistry of alkaloids, terpenoids and carotenoids • To study the Chemistry of steroids • To study the chemistry of various metabolic processes involving such biochemicals • To understand the role of such natural products in living systems

DETAILED CONTENT

MODULE-I

Terpenoids: Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, biosynthesis and synthesis of the following representative molecules: monoterpenoids, Citral, geraniol (acyclic), α-terpeneol, menthol (monocyclic). Sesquiterpenoids: farnesol (acyclic), zingiberene (monocyclic), santonin (bicyclic), diterpenoids: phytol and abietic acid.

MODULE- II

Carotenoids and Xanthophylls: General methods of structure determination of carotenes: β-carotene, α-carotene, γ-carotene, lycopene and vitamin A. Xanthophylls: spirilloxanthin, capsorubin, fucoxanthin. carotenoid acids (apocarotenoids): bixin and crocetin. bio synthesis of carotenoids

MODULE-III

Alkaloids: Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, synthesis and biosynthesis of the following: Ephedrine, coniine, nicotine, atropine, quinine and morphine.

MODULE-IV

Steroids: Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of cholesterol, androsterone, testosterone, estrone, progestrone. Biosynthesis of steroids

MODULE-V

Plant Pigments: Occurrence, nomenclature and general methods of structure determination. Isolation and

synthesis of anthocyanins (cyanin and pelargonidin), polyphenols: Flavones (chrysin), Flavonols(quercitin) and isoflavones (daidzein) coumarin, quinones (lapachol), Hirsutidin. Biosynthesis of flavonoids: Acetate pathway and shikimic acid pathway.

Books recommended:

1. Natural Products- Chemistry and Biological Significance, J. Mann, R.S. Davidson, J. B. Hobbs,D.V. Banthrope and J. B. Harborne, Longman, Essex.

2. Organic Chemistry Vol. II, I.L. Finar, ELBS.

3. Stereo selective synthesis- A Practical Approach, M. Nogradi, VCH.

4. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.

5. Chemistry, Biological and Pharmacological Properties of Medicinal Plants From the Americas, Ed.Kurt Hostettmann, M.P. Gupta and A. Marston, Harwood Academic Publishers.

6. Introduction to Flavonoids, B.A.Bohm, Harwood Academic Publishers.

7. New Trends in Natural Product Chemistry, Atta-ur-Rahman M. I. Choudhary, Harwood Academic Publishers.

8. Insecticides of Natural Origin, Sukh Dev, Harwood Academic Publishers.

SEMESTER-III

L	T	P	Credit
4	0	0	4

CHEM-EC-435: Surface Chemistry & Advanced Electrochemistry

Course Objectives	This course will demonstrate physical chemistry aspects of surface chemistry, colloids and electrochemistry relevance for applications. It helps to expose students to the developments taking place in nanotechnology and in the area of materials to find applications in modern technology.
Course Outcomes	At the end of the course, the student will be able to • Recall the concepts on adsorption isotherms, kinetics of surface reactions and thermodynamics of surfaces. • Explain importance of adsorption processes, heterogeneous catalysis, Langmuir, and BET model • Explain the properties of surface-active agents and their thermodynamics of micellization. • Understand the Debye Huckel Theory of strong electrolytes and related phenomenon of electrochemistry. • Describe the objectives of nanomaterials and their preparation by using physical and chemical methods.

DETAILED CONTENT

MODULE –I

Adsorption at solid – gas interface: Concept of ideal and non – ideal adsorption. Heat of adsorption. Types of adsorption isotherms. Single – layer adsorption – Langmuir adsorption isotherm and its derivation. Multilayer adsorption – B.E.T. theory and its kinetic derivation. Application of BET theory in its determination of surface area of the solid. Catalytic activities at surfaces: adsorption and catalysis.

MODULE –II

Adsorption at solid – liquid interface: Types of adsorptions, Gibbs adsorption equation. Isotherms of concentration and temperature change for the adsorption in solutions. Chromatographic adsorption: column chromatography, its mathematical treatment and theory. Theory of chromatography involving one solute and several solutes.

MODULE –III

Solution and Interfacial Behaviour of Surfactants: Definition and classification of surfactants. Solution properties of surfactants: micelle and reverse micelle formation, critical micelle concentration (CMC), dependence of CMC on chain length of the surfactant, micelle shape and size, factors affecting the CMC of surfactants. Thermodynamics of micelle formation, hydrophobic effect (a qualitative view only). Aggregation at high surfactant concentration (a qualitative aspect) to micelles. Surface tension and detergent. Practical application of surfactants.

MODULE –IV

Electrochemistry: Debye -Huckel theory of strong electrolytes, relaxation and electrophoretic effects, Debye – Huckel – Onsager (DHO) equation and its validity in aqueous and non-aqueous solutions. Deviations from the Onsager equation, conductance ratio. Dispersion of conductance at high frequencies (Debye – Falkenhagen effect). Dispersion of conductance at high potential gradients (Wien effect). Activity and activity coefficient, activities of electrolytes and mean ion activity coefficient. Ionic strength. The Debye – Huckel Limiting law. Electrokinetic phenomena: Electrical double layer and Stern's theory, zeta potential, Electroosmosis, Streaming potential, Electrophoresis, Influence of ions on electrokinetic phenomena (Qualitative insight).

MODULE –V

Chemistry of nanomaterials: Definition, historical perspective and classification. Effect of nanoscience and nanotechnology in various fields. Synthesis of nanoparticles by chemical and physical routes and their characterization techniques. Properties of nanostructured material: optical, magnetic and chemical properties. An overview of applied chemistry of nanomaterials.

Books Recommended:

1. Physical Chemistry of Surfaces: A.W. Admson
2. Adsorption from Solutions: J.J. Kipling
3. Micelles (Theoretical and Applied Aspects): Y. Moroi
4. Foundation of Colloid Science Vol. I and II: R.J. Hunter
5. Physical Chemistry: P.W. Atkins
6. Frontiers in Applied Chemistry: A.K. Biswas
7. Introduction to nanotechnology: Charles P.Poole, Jr. Frank, J. Owens: Wiley India

SEMESTER-IV

L	T	P	Credit
4	0	0	4

CHEM-EC-442: Chemistry of Materials

Course Objectives	To introduce the students in the area of liquid crystalline materials and solid-state material chemistry and also to impart fundamental and advance understanding on nanoscale materials, their properties and applications.
Course Outcomes	At the end of the course, the student will be able • Understand the basic concepts and formation of various supramolecular assemblies. • Know the types and structure of liquid crystals and their applications. • Learn the common and important synthesis methods, structure and composition of solid-state materials, nanomaterials and their applications in industries. • Understand the concepts, mechanism and applications of inorganic pigments. • Learn the various approaches for the synthesis

DETAILED CONTENT

MODULE-I

Multiphase Materials: Ferrous alloys, Fe-C phase transformations in ferrous alloys, stainless steels, non-ferrous alloys, properties of ferrous and non-ferrous alloys and their applications.

MODULE-II

Glasses, Polymers, Ceramics and Composites: Glasses: introduction, manufacturing, types and applications. Polymers: molecular shape, structure and configuration, crystallinity, stress-strain behaviour, Thermal behaviour, polymer types and their applications, conducting and ferro- electric polymers. Ceramics and refractories: introduction, classification, characteristics, properties, some important high refractory materials and their applications. Composites: introduction, constituents, classification, some industrially important composites, failure modes and applications.

MODULE-III

Nanomaterials and Fullerenes: Nanomaterials: Introduction, carbon nanotubes – their synthesis, properties and applications. Nanotechnology in diagnostic applications. Semiconductor quantum dots – synthesis, electronic structure and correlation of properties with size and their applications.

Fullerenes : Introduction , synthesis and purification , conductivity and superconductivity in doped fullerenes , chemistry of fullerenes . Properties – optical properties, ferromagnetism and some unusual properties of fullerenes.

MODULE-IV

Liquid Crystals: Introduction , classification , chemical constitution and liquid crystalline behavior, molecular ordering in different mesophases , identification of liquid crystals , polymeric liquid crystals , applications of liquid crystals in displays and in thermography.

MODULE-V

Superconductors: Introduction, types, properties, preparations, structure of superconductors and applications of low temperature and high temperature superconductivity.

Books recommended:

1. Solid State Physics, N. W. Ashcroft and N. D. Mermin, Saunders College Ed. 1976.

2. Principles of the Solid State, H.V. Keer, New Age International Publishers, Ed. 1993.

3. Materials Science, J.C. Anderson and K.D. Leaver, ELBS, Ed. 1971.

4. Handbook of Liquid Crystals, H. Kelker, R. Hatz and C. Schumann, Chemie Verlag, Ed. 1980.

5. Solid State Physics, J. S. Blakemore, Cambridge University Press, 1985.

6. Introduction to Material Science and Engineering, Y. W. Chung, CRC Press, Ed. 2007.

SEMESTER-IV

L	T	P	Credit
4	0	0	4

CHEM-EC-443: Advanced Organometallics

Course Objectives	The objective of this course is to teach and explain the structure and bonding aspects of simple organometallic compounds and also explain the catalyzed reaction and mechanism of organometallic compounds.
Course Outcomes	Students are able to: • Describe the studies of metal carbonyls, metal clusters, metal nitrosyls and its preparation, structures and properties. • Become familiar with some applications of organometallic compounds. • Identify the different types of organotranstion metal complexes catalyzed reactions and apply the above concepts to explain different catalytic reactions.

DETAILED CONTENT

MODULE-I

Organometallic Compounds of transition elements: Types of ligands and their classifications in organometallic compounds, 16 and 18 electron rule and its limitations. Hapto-nomenclature, synthesis, structure and bonding aspects of following organometallic compounds with carbon- π donor ligands

a) Two electron donor (olefin and acetylenic complexes of transition metals)
b) Three electron donor (π-allyl complexes of transition metals)
c) Four electron donor (butadiene and cyclobutadiene complexes of transition metals)
d) Five electron donor (cyclopentadienyl complexes of transition metals - metallocenes with special emphasis to ferrocenes)
e) Six electron donor [Benzene (arene) complex]

Fluxional and dynamic equillibria in compounds such as η^2-olefin, η^3- allyl and dienyl complexes.

MODULE-II

Homogeneous Transition metal catalysis: General considerations, reason for selecting transition metals in catalysis (bonding ability, ligand effects, variability of oxidation state and coordination number), basic concept of catalysis (molecular activation by coordination and addition), proximity interaction (insertion/inter-ligand migration and elimination, rearrangement). Phase transfer catalysis. Homogeneous hydrogenation of unsaturated compounds (alkenes, alkynes, aldehydes and ketones). Asymmetric hydrogenation.

MODULE-III

Some important homogeneous catalytic reactions:- Ziegler Natta polymerization of ethylene and propylene, oligomerisation of alkenes by aluminumalkyl, Wackers acetaldehyde synthesis,

hydroformylation of unsaturated compounds using cobalt and rhodium complexes, Monsanto acetic acid synthesis, carboxylation reactions of alkenes and alkynes using nickel carbonyl and palladium complexes. Carbonylation of alkynes (acetylene) using nickel carbonyls or palladium complexes.

MODULE-IV

Metal-metal bonding in carbonyl and halide clusters:- Polyhedral model of metal clusters, effect of electronic configuration and coordination number, structures of metal carbonyl clusters of three atoms $M_3(CO)_{12}$ (M=Fe, Ru & Os), Four metal atoms (tetrahedra) [$M_4(CO)_{12}$ {M= Co, Rh &Ir}] and octahedron of type $M_6(CO)_{16}$ [M= Co & Rh], and halide derivatives of rhenium (III) triangles, metal carbonyls involving bridged-terminal exchange and scrambling of CO group.

Transition metal-carbon multiple bonded compounds:-Metal carbenes and carbynes (preparation, reactions, structure and bonding considerations). Biological applications and environmental aspects of organometallic compounds, organometallic compounds in medicine, agriculture and industry.

MODULE-V

Stability of Coordination Compounds- Stability constants, stepwise formation constants, overall formation constants, relationship between stepwise and overall formation constants, difference between thermodynamic and kinetic stability.

Determination of stability constants by:

(ii) Spectrophotometric methods (Job's method, mole ratio and slope ratio method).
(ii) Bjerrum's method
(iii) Leden's method
(iv) Polarographic method

Factors affecting the stability constants (with special reference to metal and ligand ions).

Books recommended:

1. *Principles of organometallic compounds – Powell*
2. *Organometallic chemistry (an Introduction) – Perkin and Pollar*
3. *Organometallic chemistry – Parison*
4. *Advanced Inorganic Chemistry - Cotton and Wilkinson*
5. *Organometallic Chemistry-R.C.Mehrotra*
6. *Organometallic compounds of Transition Metal-Crabtree*
7. *Chemistry of the Elements - Greenwood and Earnshaw*
8. *Inorganic Chemistry - J.E.Huheey*
9. *Homogeneous transition metal catalysis - Christopher Masters*
10. *Homogeneous Catalysis - Parshall*
11. *Principles and Application of HomogeneousCatalysis - Nakamura and Tsutsui*
12. *Progress in Inorganic Chemistry Vol. 15 - Lipard. (Transition metal clusters - R.B.King)*
13. *Organotransition metal chemistry by S.G.Davis, Pergamon press 1982.*
14. *Principles and applications of organotransition metal chemistry by Ccollmen and Hegden*

SEMESTER-IV

L	T	P	Credit
4	0	0	4

CHEM-EC-444: Inorganic Spectroscopy

Course Objectives	The aim and objective of this course is to learn various techniques of spectrometric identification of inorganic compounds and to characterize inorganic compounds by applying various techniques together.
Course Outcomes	By the end of the course students will be able to: • Interpret IR spectroscopy. Explain basic principles of IR spectroscopy. Arrange components of IR spectroscopy device. Explain working principles and taking spectrum of IR spectroscopy device. • Will be able to interpret NMR spectroscopy. Explain basic principles of NMR spectroscopy. Explain sample preparation procedure in NMR spectroscopy. • Explain working principles, taking spectrum and outline of NQR, MB and ESR spectroscopy device. Will be able to interpret elemental analysis technique.

DETAILED CONTENT

MODULE-I

Infrared Spectroscopy: Theory of IR absorption, types of vibrations, observed number of modes of vibrations, intensity of absorption bands, theoretical group frequencies, factors affecting group frequencies and band shapes (Physical state, vibrational coupling, electrical effects, resonance, inductive effects, ring strain) vibrational-rotational fine-structure. Experimental method. Application of IR to the following:

i) Distinction between

a) Ionic and coordinate anions such as NO_3^-, SO_4^{2-} and SCN^-

b) Lattice and coordinated water.

ii) Mode of bonding of ligands such as urea, dimethylsulphoxide and hexamethylphosphoramide.

MODULE-II

Nuclear Magnetic Resonance Spectroscopy:- Introduction to nuclear magnetic resonance, chemical shift, mechanism of electron shielding and factors contributing to the magnitude of chemical shift, nuclear overhauser effect, double resonance, chemical exchange, lanthanide shift reagents and NMR spectra of paramagnetic complexes. Experimental technique (CW and FT).

Stereochemical non-rigidity and fluxionality: Introduction, use of NMR in its detection, its presence in trigonal bipyramidal molecules (PF_5), Systems with coordination number six ($Ti(acac)_2Cl_2$, $Ti(acac)_2Br_2$, $Ta_2(OMe)_{10}$,).

MODULE-III

Nuclear Quadrupole Resonance Spectroscopy: Basic concepts of NQR (Nuclear electric quadrupole

moment, electric field gradient, energy levels and NQR frequencies). Effect of magnetic field on spectra. Factors affecting the resonance signal (Line shape, position of resonance signal). Relationship between electric field gradient and molecular structure. Interpretation of NQR data, structural information of the following: PCl_5, $TeCl_4$, Na^+GaCl^{4-}, BrCN, HIO_3 and hexahalometallates

MODULE-IV

Mossbauer Spectroscopy: Introduction, principle, conditions for Mossbauer spectroscopy, parameters from Mossbauer spectra, isomer shift, electric quadrupole interactions. Magnetic interactions. MB experiment. Application of MB spectroscopy in structural determination of the following:

i) High spin Fe(II) and Fe(III) halides FeF_2, $FeCl_2.2H_2O$, FeF_3, $FeCl_3.6H_2O$. Low spin Fe(II) and Fe(III) Complexes- Ferrocyanides, Ferricyanides, Prussian Blue.

ii) Iron carbonyls. $Fe(CO)_5$, $Fe_2(CO)_9$ and $Fe_3(CO)_{12}$

iii) Inorganic Sn(II) and Sn(IV) halides.

MODULE-V

Electron Spin Resonance Spectroscopy: Introduction, similarities between ESR and NMR. Behaviour of a free electron in an external magnetic field. Basic principle of an electron spin resonance spectrometer, presentation of the spectrum. Hyperfine coupling in isotropic systems.

(methyl, benzene and naphthalene radicals). Factors affecting the magnitude of g-values. Zero field splitting and Kramer's degeneracy. Line width in solid state ESR, double resonance technique in e.s.r. (ENDOR), experimental method. Applications of ESR to the following:

1. Bis-Salicylaldiimine - Copper –II
2. $CuSiF_6.6H_2O$ & $(NH_3)_5Co\text{-}O.Co(NH_3)_5$

Books recommended:

1. *Physical methods in Inorganic Chemistry - R.S.Drago.*
2. *Modern Optical methods of Analysis - Eugens D.Olsen*
3. *Infrared spectra of Inorganic and coordination compounds - Kazuo Nakamoto*
4. *Introduction to Chemistry -Donald L.Pavia and G.M.Lampman.*
5. *Fundamentals of Molecular Spectroscopy-C.N.Banwel*
6. *Spectroscopy in Inorganic Chemistry - Rao & Ferraro Vol I & II*
7. *Advances in Inorganic and Radiation Chemistry Vol 6 & 8.*
8. *Quarterly reviews Vol 11 (1957)*
9. *Progress in Inorganic Chemistry Vol 8*
10. *Organic Spectroscopy-W. Kemp*

SEMESTER-IV

L	T	P	Credit
4	0	0	4

CHEM-EC-445: Catalysis and Green Chemistry

Course Objectives	The objectives of this course are to introduce fundamental understanding of catalysis and green chemistry one of the central tools in green chemistry. Students will be furnished with the necessary tools to evaluate synthetic protocols and industrial processes, and their impact in the environment and human health. The students will also be exposed to the development of latest technologies and methodologies for environmentally benign methods which are being practiced in industry.
Course Outcomes	After completing this course, student will be able to – • explain how green chemistry relates to problems of societal concern. • Analyze a process and identify how it can be made more environmentally friendly/sustainable. - make connections between previous coursework and integrate with green chemistry and sustainability concepts. • Classify catalysts and catalytic reactions in important groups. - explain the contribution of catalysis in chemical industry and in the development of environmentally friendly chemical processes. - analyze and decide best choice of the catalyst for a given catalytic reaction.

DETAILED CONTENT

MODULE-I

Fundamentals: Catalyst, activation energy concept, types of catalysis, comparison of homogeneous and heterogeneous catalysis, enzyme catalysis, green catalysis, nanocatalysis, autocatalysis, phase transfer catalysis. Promoters and poison.

MODULE-II

Homogeneous and heterogeneous catalysis: Noyori asymmetric hydrogenation, metal mediated C-C and C-X coupling reactions, Heck, Stille, Suzuki, Negishi, Sonogashira and Ullmann coupling reactions. Directed orthometalation, metal (Rh, Ir) catalysed C-H activation reactions.

Adsorption isotherms, surface area, pore size and acid strength measurements, porous solid catalysis by semiconductors and solid acid supported metal catalysts, catalyst preparation, deactivation and regeneration model catalysts, hydrogenation of carbon monoxide and hydrocarbon conversion.

MODULE-III

Photocatalysis: Porphyrins, phthalocyanines and semiconductors as photo catalysts in photocatalysis reactions. Generation of hydrogen by photo catalysts. Photocatalytic break down of water and harnessing solar energy. Photocatalytic degradation of dyes, environmental applications.

MODULE-IV

Introduction, principle and concepts of green chemistry: Need for green chemistry, inception and evolution of green chemistry; twelve principles of green chemistry with their explanations and examples; designing a green synthesis using these principles; green chemistry in day to day life.

MODULE-V

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.

Books recommended:

1. *Green Chemistry and Catalysis, Roger Arthur Sheldon, Isabel Arends, and Ulf Hanefeld, Wiley, 2007.*
2. *Green Chemistry Theory and Practice P.T Anasts and J. C. Warner, Oxford University Press, 2000.*
3. *Understanding Organometallic Reaction Mechanisms and Catalysis Computational and Experimental Tools, Valentin P. Ananikov, Weinheim, Bergstr Wiley-VCH 2014.*
4. *Principles and Practice of Heterogeneous Catalysis, John Meurig Thomas, W. John Thomas, Wiley-VCH 2015.*
5. *Handbook of Green Chemistry, Volume 1. Green Catalysis, Homogeneous Catalysis. Anastas P.T., Crabtree R.H. (eds.), Wiley-VCH 2013.*

SEMESTER-IV

L	T	P	Credit
4	0	0	4

CHEM-EC-446: Synthetic Strategies

Course Objectives	The aim and objective of this course is to give knowledge about selective synthesis, in particular for stereoselective synthesis; to describe basic chemo-, regio- and stereochemical concepts; explain the selectivity observed in chemical reactions; make students familiar with the methods for selective synthesis of simple organic compounds, also containing stereogenic elements; suitable reagents for selective transformations; prepare organic compounds using advanced synthetic methodology; explain the basic mechanism of oxidation in organic compounds; describe the reagents which cause oxidation in various compounds; make familiar with the two types of reduction reactions like complete reduction and selective reduction; identify the reagents that cause selective and complete reduction and describe stereochemical problems related to chemical transformations, important stereochemical like chiral reagents and catalysts and Organometallic reaction mechanisms and its applications. In addition, this course will make the students familiar with disconnection approach for organic synthesis.
Course Outcomes	The students will be able to apply • The knowledge and understand essential facts, concepts, principles and theories relating to retrosynthetic analysis for the synthesis of organic target molecules. • Emphasize the role of various organometallic complexes in Organic Synthesis • Understand the methodological concept of connection disconnection in organic synthesis.

DETAILED CONTENT

MODULE-I

Organic Reagents: Reagents in organic synthesis: Willkinson catalyst. Lithium dialkyl cuprates (Gilman's reagents). Lithium diisopropylamide (LDA),1,3-Dithiane (Umpolung) Dicyclohexylcarbobiimide (DCC), and Trimethylsilyliodide, DDQ, SeO_2, Baker yeast, Tri-n-butyltinhydride, nickel tetracarbonyl, Trimethylchlorosilane.

MODULE-II

Oxidations: Introduction, Different oxidative process. aromatiztion of six membered ring, dehydrogenation yielding C-C double bond, oxidation of alcohols, oxidation involving C-C double bond, oxidative cleavage of ketones, aldehydes and alcohols, double bonds and aromatic rings, ozonolysis, oxidative decarboxylation, Bisdecarboxylation, oxidation of methylene to carbonyl, oxidation of olefines to aldehydes and ketones.

MODULE -III

Reductions: Introduction, different reductive processes. Reduction of carbonyl to methylene in aldehydes and ketones, reduction of nitro compounds and oximes, reductive coupling, bimolecular reduction of

aldehydes or ketones to alkenes, metal hydride reduction, acyloin ester condensation, Cannizzaro reaction, Tishchenko reaction, Willgerodt reaction .

MODULE-IV

Rearrangements: General mechanistic considerations-nature of migration, migratory aptitude, memory effects. A detailed study of the following rearrangements: Benzil-Benzilic acid, Favorskii, Arndt-Eistert synthesis, Neber, Backmann, Hofmann, Curtius, Schmidt, Benzidine, BaeyerVilliger, Shapiro reaction, Witting rearrangement and Stevens rearrangement.

MODULE-V

Disconnection Approach: An introduction to synthons and synthetic equivalents, disconnection approach, functional group inter-conversions, the importance of the order of events in organic synthesis, one group C-X and two group C-X disconnections, chemoselectivity, reversal of polarity cyclisation reactions, amine synthesis. Protecting groups: principle of protection of alcohol, amine, carbonyl and carboxyl groups. One group C-C disconnection: alcohols and carbonyl compounds, regioselectivity. Alkene synthesis, use of acetylenes in organic synthesis.

Books recommended:

1. *Designing Organic Synthesis, S. Warren, Wiley.*
2. *Organic Synthesis- Concept, Methods and Starting Materials, J. Fuhrhop and G. Penzillin, VerlageVCH.*
3. *Some Modern Methods of Organic Synthesis, W. Carruthers, Cambridge Univ. Press.*
4. *Modern Synthetic Reactions, H.O. House, W. A. Benjamin.*
5. *Advanced Organic Chemistry-Reactions Mechanisms and Structure, J. March, Wiley.*
6. *Principles of Organic Synthesis, R. Norman and J.M. Coxon, Blakie Academic and Professional.*
7. *Advanced Organic Chemistry Part-B, F.A. Carey and R. J. Sundburg, Plenum Press.*
8. *Organomettalic Chemistry-A Unified Approach, R.C. Mehrotra, A. Singh.*

SEMESTER-IV

L	T	P	Credit
4	0	0	4

CHEM-EC-447: Medicinal Chemistry

Course Objectives	The aim and objective of this course is to familiarize students with the basic concept of Medicinal Chemistry. Emphasis will be made on the SAR of various drugs such as Antimicrobial, antihelmenthics, Psycotropic drugs and their mode of actions. The commercial synthesis of representative of such drugs will also be discussed.
Course Outcomes	At the end of the course, the student will be able to • Understand the need of Medicinal Chemistry in curing various ailments. • Study the concept of Antimicrobial, Psycotropic Drugs and cardiovascular drugs. • Study the SAR of Antimicrobial and Psycotropic drugs. • Understand the total synthesis of Antimicrobial and other drugs. • Understand the various diseases cured by Antimicrobial, Anticonvulsants and Diuretics drugs.

DETAILED CONTENT

MODULE-I

Drug Design: Development of new drugs, procedures followed in drug design, concepts of lead compound and lead modification, concepts of prodrugs and soft drugs, structure-activity relationship (SAR), factors affecting bioactivity, resonance, inductive effect, isosterism bio-isosterism, spatial considerations. Theories of drug activity: occupancy theory, rate theory, induced fit theory. Quantitative structure activity relationship. History and development of QSAR. Concepts of drug receptors.Elementary treatment of drug receptor interactions. Physico-Chemical parameters: lipophilicity, partition coefficient, electronic ionization constants, steric, Free-Wilson analysis, Hansch analysis relationships between Free-Wilson and Hansch analysis.

MODULE-II

Pharmacokinetics and Pharmacodynamics: Pharmacokinetics: Introduction to drug absorption, disposition, elimination using pharmacokinetics.Important pharmacokinetic parameters in defining drug disposition and in therapeutics. Mention of uses of pharmacokinetics in drug development process.

Pharmacodynamics: Introduction, elementary treatment of enzyme stimulation, enzyme inhibition, sulphonamides, membrane active drugs, drug metabolism, xenobiotics, biotransformation. Significance of drug metabolism in medicinal chemistry.

MODULE-III

Antibiotics and Antiinfective Drugs: Antibiotics: Structure, SAR and biological action of antibiotics. Examples: penicillin: penicillin G, penicillin V, ampicillin, amoxycillin, chloramphenicol, cephalosporin, tetracycline and streptomycin.

Sufonanmides: Structure, SAR and mode of action of sulfonamides, sulfonamide inhibition and probable mechanisms of bacterial resistance to sulfonamides. Examples: sulfodiazine, sulfofurazole, acetyl sulfafurazole, Sulfagnanidine, Phthalylsulfo acetamide, Mafenide. Sulphonamide related compounds Dapsone. Local antiinfective drugs: Introduction and general mode of action. Examples: sulphonamides, furazolidone, nalidixic acid, ciprofloxacin, norfloxacin, chloroquin and primaquin

MODULE-IV

Psychoactive Drugs: Introduction, neurotransmitters, CNS depressants and stimulants. SAR and Mode of actions. Central Nervous System Depressant: General anaesthetics.
Sedatives & Hypnotics: Barbiturates and benzodiazepines.
Anticonvulsants: barbiturates, oxazolidinediones, succinimides, phenacemide and Benzodiazepines.
Psycotropic Drugs: The neuroleptics (Phenothiazines and butyrophenones), antidepressants (monoamine oxidases inhibitors and tricyclic antidepressants) and anti-anxiety agents (Benzodiazepines).
Central Nervous System Stimulants: Strychnine, purines, phenylethylamine, analeptics, indole ethylamine derivatives,

MODULE-V

Therapeutic Agents, SAR and Their mode of Actions: Antineoplastic agents: Cancer chemotherapy, role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic, antiobiotics and mitotic inhibitors. Biological action of mechlorethamine, cyclophosphamide, melphalan, uracil, and 6-mercaptopurine.
Cardiovascular Drugs: Antihypertensive and hypotensive drugs, antiarrrhythemic agents, vasopressor drug direct acting arteriolar dilators. Biological action of methyldopa, propranolol hydrochloride, amyl nitrate, sorbitrate, verapamil, atenolol.
Antihistaminic agents: Ethylene diamine derivatives, amino alkyl ether analogues, cyclic basic.
Antifertility agents: General antifertility agents.
Diuretics: Mercurial diuretic, non-mercurial diuretics (Thiazides, carbonic-anhydrase inhibitors, xanthine derivatives, pyrimidine diuretics and osmotic diureteics

Books recommended:

1. *An Introduction to Medicinal Chemistry, Graham L. Patrick.*
2. *Medicinal Chemistry: Principles and Practice Edited by F.D. King.*
3. *Textbook of Organic Medicinal and Pharmaceutical Chemistry, Edited by Charles O. Wilson, Ole Gisvold, Robert F. Doerge.*
4. *Introduction to Medicinal Chemistry, Alex Gringuage.*
5. *Principles of Medicinal Chemistry, William O. Foye, Thomas L. Lemice and David A. Williams.*
6. *Introduction to Drug Design, S.S. Pandeya and J. R. Dimmock, New Age International.*
7. *Burger's Medicinal Chemistry and Drug Discovery, Vol-1 (Chapter-9 and Ch-14), Ed. M.E. Wolff, John Wiley.*
8. *Goodman and Gilman's Pharmacological Basis of Therapeutics, Mc Graw-Hill.*
9. *The Organic Chemistry of Drug Design and Drug Action, R.B. Silverman, Academic Press.*
10. *Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley.*

SEMESTER-IV

L	T	P	Credit
4	0	0	4

CHEM-EC-448: Polymer Chemistry

Course Objectives	Students will be introduced to the field of polymer chemistry, synthetic methods and characterization.
Course Outcomes	Students will be able to use the understanding gained for the synthesis and characterization of polymer materials for designing novel polymeric materials for applications.

DETAILED CONTENT

MODULE - I

Historical background, types, classification and importance of polymers, chemical and geometrical structure, physical state and thermal transition: crystalline melting temperature, Tm and glass transition temperature, Tg. Properties of polymers: thermal, mechanical, rheological and electrical properties. Applications and future trends of polymers

MODULE - II

Step polymerization, chain polymerization including carbonyl polymerization, ionic polymerization, co-ordination polymerization, atom transfer free radical polymerization,supramolecular polymerization, ring opening polymerization, metathesis polymerization, group transfer polymerization; emulsion polymerization, chain copolymerization. Reactivity ratio and control of molecular weight in polymerization.

MODULE - III

Average molecular weight concept, Number average, weight average, viscosity average molecular weights. Polydipersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weights. End group analysis, viscosity, light scattering, osmotic and ultrantracentrifugation methods, fractionation of polymers, Gel permeation chromatography (GPC). Chemical analysis of polymers: Spectroscopic methods, X-ray diffraction study, microscopy,
thermal analysis.

MODULE – IV

Chain conformation, kinetic chain length; molecular dimensions in solution, solubility of polymers, solubility parameters, transfer process, lattice theory, thermodynamics of polymer dissolution; ΔH, ΔS and ΔG of mixing; Flory–Huggins theory, thermodynamics of dilute polymer solutions, , $\chi 1$ and θ-temperature.

MODULE - V

Chemical degradation, physical degradation, ageing, crazing, degradation by micro organisms, Biodegradable polymers, Mechanism of degradation, secondary chain reaction, Self reaction, depolymerisation, metal catalysed degradation, Thermal oxidation, Photooxidation, Mechanical degradation, Degradation by ionizing radiation, ozone attack. Degradation of special polymers: Polyolefins, PVC, PS, PMMA. Stabilization: Chain breaking antioxidants, bound antioxidants, Radiation protection, Stabilization against biodegradation.

Books Recommended:

1. Kaim, W.; Schwederski, B.; Klein, A., Bioinorganic Chemistry-Inorganic Elements in the Chemistry of Life: An Introduction and Guide, 2nd Ed., John Wiley & Sons, West Sussex (2013).
2. Bertini, I.; Gray, H. B.; Lippard, S. J.; Valentine, J. S., Bioinorganic Chemistry, Viva Books, New Delhi (2007).
3. Housecroft, C. E; Sharpe, A. G., Inorganic Chemistry, 5th Ed., Pearson Education, Essex (2018).
4. Atkins, P.; Overton, T.; Rouke, J.; Weller, M.; Armstrong, F.; Hagerman, M., Shriver Atkins's Inorganic Chemistry, 6th Ed., Oxford University Press, New Delhi (2015).
5. Huheey, J. E.; Keiter, E. A.; Keiter, R. L.; Medhi, O. K., Inorganic Chemistry: Principles of Structures and Reactivity, 4th Ed., Pearson Education India, New Delhi (2006).

SEMESTER-IV

L	T	P	Credit
4	0	0	4

CHEM-EC-449: Organometallic and Heterocyclic Chemistry

Course Objectives	Students will be introduced to the chemistry of organo transition metals complexes, their role in organic synthesizes and different heterocyclic rings. The student will be able to learn nomenclature, structure, properties, syntheses, and reactions of the simple small, 3, 4, 5, 6, 7 and large membered heterocyclic rings.
Course Outcomes	Students will be able to • have a good overview of the fundamental principles of organotransition-metal chemistry and know how chemical properties are affected by metals and ligands • know important applications of organometallic oomogeneous/heterohenous catalysis in the production of large-scale (bulk) and smaller-scale (fine chemicals) production • understand fundamental reaction types and mechanisms and how to combine these to understand efficient catalytic processes • At the successful completion of the course the student will have knowledge about the structures, syntheses, reactions, and properties of the major classes of heterocyclic compounds.

DETAILED CONTENT

MODULE - I

Chemistry of Organotransition metal complexes: General introduction. 18- and 16-Electron rules. General rules.

Complexation and De-complexation Reactions: s-Bonded systems including h1 ligands. pBonded systems involving dihapto to octa hapto ligands such as- olefins, acetylenes, allylmoieties, butadiene, cyclobutadiene, arenes, cyclopenta, cyclohexa and cycloheptadienylmoieties; cyclohepta, cyclooctatrienes, and cyclooctatetraene moieties. Use of organotransition metal complexes as protecting and stabilizing groups: Protection of olefins, acetylenes and dienes. Stabilization of cyclobutadines and norbornadienones. Organometallics as electrophiles and nucleophiles: Nucleophilic addition to h2, h5 and h6complexes. Electrophilic addition to h4, h6 and carbene complexes.

MODULE - II

Organometallics in coupling and cyclization reactions: Coupling and cyclization of organic nucleophiles with olefins (including Heck reaction), and coupling of olefins with acetylenes (including Felkin's reaction).

Organometallics in isomerization, oxidation and reduction reactions: Isomerization of olefins, allylic alcohols and allylic ethers. Oxidation of olefins (including Wacker's process and epoxidation) and reduction of olefins and α,β-unsaturated compounds (including Wilkinson's reaction).

MODULE - III

Carbonylation reactions: Use of zirconium complexes in the synthesis of esters, acids, aldehydes or acyl halides from alkyl halides and in the hydroformylation of olefins and dienes. Use of iron complexes for the insertion of CO group into organic molecules such as dienes, alkyl halides, and vinyl epoxides. Use of cobalt complexes in the synthesis of ketones from epoxides, lactones from allylic alcohols and in the hydroformylation of olefins. Use of palladium complexes for the carbonylation of alkyl halides, dienes and allenes.

Application of the following organometallics in Organic Synthesis: Organozincs, Organolithiums, Organo copper, Organoseleniums, Organotelluriums, Organoaluminiums, Organosilicons, Organotins and Organomercurials

MODULE – V

Small ring heterocycles: Properties and reactions of 3- and 4- membered heterocycles:- oxiranes, thiranes, aziridines, azetidines, oxetanes and thietanes. Benzo-fused heterocycles: Synthesis and reactions of benzofurans, benzothiophenes,benzoxazoles, benzothiazoles and benzimidazoles. Six-membered heterocycles with two or more heteroatoms: Synthesis of Diazines, triazines, tetrazines and thiazines.

MODULE - V

Seven and large membered heterocycles: Synthesis and reactions of azepanes, oxepines, thiepines, diazepines, thiazepines, azocines, diazocines, dioxocines and dithiocines. Heterocycles containing P, As, Sb and Bi: Synthesis of 5- and 6- membered heterocycles with P, As, Sb and Bi. Mesoionic compounds: General classification, chemistry of some important meso-ionic heterocycles of type-A and type-B and their applications.

Books Recommended:

1. Organometallic Chemistry, R. C. Mehrotra and A. Singh, Wiley Eastern, 1991.
2. The Organometallic Chemistry of the transition metals, R. H. Crabtree, 1988.
3. Principles and application of the organotrnsition metal chemistry, J. P. Collman, L. S. Hegedus, University Science books, 1980.
4. An introduction to Organometallic Chemistry, A. W. Parkins and R. C. Poller, Macmillan, 1986.
5. Modern Synthetic Reactions, H. O. House, W.A. Benjamin, California, 2nd Edition 1972.
6. Organometallics, Vol. 1 & 2, M. Bochmann, Oxford Chemistry primers, Oxford University Press, 1994.
7. Advanced Organic Chemistry, J. March, 4th Edition. John Wiley, 2008.
8. Organotransition metal chemistry, S. G. Davies, Pergamon Press, Oxford, 1982.
9. Heterocyclic Chemistry, Vols. 1-3, R. R. Gupta, M. Kumar and V. Gupta, Springer Verlag.
10. The Chemistry of Heterocycles, T. Eicher and S Hauptimann, Thieme.
11. Heterocyclic Chemistry, J. A. Joule, K. Mills and G. F. Smith, Chapman and Hill.
12. Heterocyclic Chemistry, T. L. Gilchrist, Longman Scientific Tech.
13. Contemporary Heterocyclic Chemistry, G. R. Newkome, and W. W. Paudler, Wiley-Inter Science.
14. An introduction to Heterocyclic Compounds, R. M. Acheson, John Wiley.
15. Comprehensive Heterocyclic Chemistry, A. R. Katritzky and C. W. Rees, Eds. Pergamon Press.
16. Stereochemistry of Organic Compounds, D Nasipuri, New-Age International, 1999

SEMESTER-IV

L	T	P	Credit
4	0	0	4

CHEM-EC-450: Solid State Chemistry

Course Objectives	The objective of this course is to equip students with the conceptual knowledge of solid-state chemistry. It helps students to understand different properties of solids that are explained for metals, semiconductors, insulators and superconductors.
Course Outcomes	By the end of this course student will be able to • Describe X-ray and electron diffraction and to analyze information from various structure characterization methods and utilize powder X-ray diffraction data for phase identification. • Describe the importance and properties of defects in solid. Explain the free election and band theories of solids. • Illustrate the electrical, electronics, optical, dielectric and thermal properties of solids. • Design and development of solid materials with pre-required properties based on the structure of solids. • Understand the phenomenon of superconductivity and superconductors. • Describes general principles and classified preparation of solids by various methods such as solid-state reactions, preparation and properties of thin films.

DETAILED CONTENT

MODULE - I

X- ray diffraction: X-rays Diffraction by crystals. The Laue equations and Bragg's law. Indexing of powder and crystal photographs. Determination of Bravais lattice, point group and space group. Electron diffraction: the scattering of electron by gases (Wierl equation), visual method, radial distribution method. Limitations and applications of electron diffraction.

MODULE - II

Bonding in crystals: Ionic crystals, lattice energy of ionic crystals, metallic crystals. Imperfections: point defects (Schottky and Frankel defects). Thermodynamic derivation of these defects. Theories of bonding: Free electron theory; quantum approach, Fermi – Dirac statistics. Zone theory; quantum approach, allowed energy zones, Brillouin zones, k – space, Fermi surfaces and density states.

MODULE - III

Properties of crystals: Electrical properties of metals: conductors and non – conductors, conductivity in pure metals, Hall effect. Thermal properties: theories of specific heat. Electrical properties of semiconductors: band theory, intrinsic and extrinsic semiconductors, electrons and holes, temperature dependence and mobility of

charge carriers. Optical properties: absorption spectrum, photoconductivity, photovoltaic effect and luminescence, refraction birefringence and color centre. Dielectric properties: piezoelectricity, ferro electricity, ionic conductivity and electric breakdown.

MODULE – IV

Superconductivity: experimental survey, occurrence of superconductivity, destruction of superconductivity by magnetic fields (Meissner effect). Thermodynamic effects of superconducting species (entropy, thermal conductivity and energy gap). Quantum tunnelling. Theoretical survey (thermodynamics of superconducting transition, London equation, coherence length). BCS theory of superconductivity.

MODULE - V

Solid State Reactions: General principles: experimental procedures, kinetics of solid-state reactions, vapour phase transport methods, intercalation or ion exchange reaction, electrochemical reduction methods, preparation of thin films, growth of single crystal, high pressure and hydrothermal method.

Books Recommended:

1. Introduction to Solids: Azaroff
2. Solid State Chemistry and its applications: West
3. Solid State Chemistry: Charkrabarty
4. Solid State Chemistry: N.B. Hannay
5. Solid State Physics: Kiittal
6. Polymer Science: P. Bhadur and N.V. Sastry

SEMESTER-IV

L	T	P	Credit
4	0	0	4

CHEM-EC-451: Advanced Quantum Chemistry

Course Objectives	To impart knowledge regarding basics of Quantum mechanics, eigen values, wave equations and their theory and applications for solving various problems in physical chemistry.
Course Outcomes	At the end of the course, the student will be able to • Understand the need for quantum mechanical formalism and basic principles. • Appreciate the importance and implication of generalized uncertainty principle in quantum mechanics. • Solve the eigen value problems. • Have a better understanding of the mathematical foundations of angular momentum of microscopic particles. • Apply Schrodinger wave equation and approximation methods for problem solving in quantum mechanics. • Rationalize the concept of bonding in conjugated polyenes.

DETAILED CONTENT

MODULE - I

Perturbation method: Time – independent perturbation theory. Non – degenerate perturbation theory; First order correction to the energy and wave-function. Application to particle in one-dimensional box, ground state helium atom (without spin consideration) and harmonic oscillator. Perturbation theory for degenerate states, first order perturbation for degenerate states.

MODULE - II

Variation method: Theory for ground and excited state energy and wave function. Linear and non-linear variation functions. Application to ground state hydrogen and helium atoms, one – dimensional box and harmonic oscillator. Fermi Golden Rule. Radiation–matter interaction (induced emission and absorption of radiation). Einstein's transition probabilities.

MODULE - III

Quantum – mechanical concept of multielectron atoms: Slater determinants for n-electron atoms. Hartree and Hartree – Fock self – consistent field (HFSCF) method. Roothaan's method. Correlation energy (CE) and configuration interaction (CI). Koopmann's theorem. Basic idea of Density functional theory (DFT). Kohn – Sham equations.

MODULE – VI

Quantum – mechanical treatment of molecular systems: The Born Oppenheimer approximation and its formulation. The linear combination of atomic orbital (LCAO)-approximation. Molecular Orbital Theory (MOT): MOT of H_2 and H_2^+, MOT with configuration interaction (CI). Valence bond theory / Heitler – London treatment: Valence – bond treatment of H_2 and H_2^+.

MODULE – V

Quantum – mechanical treatment: Quantum – mechanical treatment of Π - electron systems/ Free electron molecular orbital (FEMO) theory. The Π - electron approximation. The Huckel –Molecular Orbital Theory (HMOT) for systems. Huckel calculations for ethylene, allyl systems, 1,3- Butadiene, cyclobutadiene and benzene. Calculation of electron density, charge distribution and bond orders.

Books Recommended:

1. Quantum Chemistry An Introduction: H.L. Strauss
2. ntroductory Quantum Chemistry: A.K. Chandra
3. Quantum Chemistry: D.A. McQuarri
4. Quantum Chemistry: I.N. Levine
5. Molecular Quantum Mechanics: P.W. Atkins
6. Elementary Quantum Chemistry: F.L. Pilar
7. Introductory Quantum Chemistry: S.R. LaPaglia
8. Fundamental Quantum Chemistry: T.E. Peacock

SEMESTER-IV

L	T	P	Credit
4	0	0	4

CHEM-EC-452: Biophysical Chemistry

Course Objectives	The objective of this course is to provide exposure to the students of structure, function, folding and dynamics of cell membrane and proteins.
Course Outcomes	On completion of the course, the student should be able to: • Account for the different biomolecular interactions that are important for the formation of structures in biological systems and for how thermodynamic parameters can be measured. • Account for structures and functions of biological membranes, as well as model systems and relevant methods for the study of these structures and functions. • Explain and apply methods for the determination of functional molecular mass of biological macromolecules in solution as well as determination of equilibrium - and rate constants for macromolecule-ligand interactions. • Explain all types of inter-and intra-molecular interactions and their contribution to the native conformation of biomolecules.

DETAILED CONTENT

MODULE - I

Cell membrane and its structure: The cell membrane, structure and functions of proteins, enzymes, DNA and RNA in living systems. Helix coil transition. Lipids in biological membranes, phospholipids, sphingolipids, glycolipids, cholesterol, gangliosides, lipoproteins, types and arrangements of proteins in membranes. Danielli and Davson model, Fluid Mosaic Model, permeability of cell membrane.

Bio-Energetics: Thermodynamic Considerations, standard free energy change in bio-chemical reactions, exergonic, endergonic reactions, High energy molecules, hydrolysis of ATP and its synthesis from ADP.

MODULE - II

Biopolymers: Statistical mechanics in biopolymers chain configuration of macromolecules, statistical distribution end – to - end dimensions, Polypeptide, protein structures and protein folding. Calculation of average dimensions for various chain structures.

Neuro biophysics: Neurons, synapse, physics of membrane potential. Neurotransmitters: Serotonin, GABA.

MODULE - III

Mechanism of Membrane Transport: Transport through cell membrane, active and passive transport systems (chemi-osmotic theory). Irreversible thermodynamic treatment of membrane transport, Donnan effect in osmosis, its dependence on pH difference across the membrane.

Bio-mechanics: Striated muscles, contractile proteins, mechanical properties of muscles and role of calcium.

MODULE – VI

Biomolecular Interactions: Interactions between biomolecules (proteins), interaction of biomolecules with small ligands, independent ligand binding sites, the Scatchard plot. Forces involved in the stability of proteins; hydrophobic interactions, hydrogen bonding, electrostatic interactions, electron delocalization, van der Waal's forces weak interactions crucial to macromolecular structure and function, blood –the buffering system.

MODULE – V

Protein molecules: Protein sequence and structure (primary structure), secondary structure, Ramachandran plot, (α-helix, β-strand, β-sheet, turns and loops), torsion angles, tertiary structure (ion-ion, ion-dipole and dipole-dipole interactions), quaternary structure, Globular and fibrous proteins, Structure of haemoglobin and myoglobin and their physiological roles, Protein folding, refolding and misfolding, Chaperones and chemical factors (Intra and intermolecular interactions) leading to folding/refolding/misfolding, Brain diseases associated with proteins.

Books Recommended:

1. Physical Chemistry of Macromolecules: S.F.Sun
2. The Enzyme Molecules: W. Ferdinand
3. Outlines of Biochemistry: E.E. Conn and P.K. Stumph
4. Biochemistry: Zubay
5. Principles of Biochemistry: A.I. Leninger
6. Physical Biochemistry: D. Friefelder
7. Biophysics: Volkenstein
8. Biophysical Chemistry (Vol. I-III): Schimell and Cantour
9. Biophysics: Vasantha Pattabhi, N.Gautam
10. Biophysical Chemistry: Gurtu &Gurtu

SEMESTER-IV

L	T	P	Credit
4	0	0	4

CHEM-EC-453: CHEMISTRY OF MACROMOLECULES

Course Objectives	This course aims at acquainting the students the knowledge of basic concepts of chemistry of macromolecules. A complete packet of knowledge of the kinetics, thermodynamics of polymerization, various techniques of determination of molecular mass, physical properties and applications of polymers in various fields of life will be provided to the students. Various factors affecting the structure and properties of polymers will be discussed in detail which makes students aware of the things to be considered while preparing polymers commercially.
Course Outcomes	On completion of the course, the student should be able to: • Interpret and explain various factors affecting structure and properties of macromolecules. • Select the appropriate polymerization mechanism for a given monomer, to describe the experimental methods for molecular weight characterization and for determination of the main thermal transitions, and to correlate thermal and mechanical properties with chemical structure. • Pursue their career objectives in higher education, scientific research and teaching.

DETAILED CONTENT

MODULE - I

Macromolecules and their physical properties: Introduction to Macromolecules, classification and importance. Synthetic and natural polymer. Polymerization (condensation and addition reactions), effect of temperature and pressure on chain polymerization. Molecular forces and chemical bonding in macromolecules and their effects on the physical properties. Polymer solutions, criteria for polymer solubility, conformations of dissolved polymer chains. The amorphous, semicrystalline and crystalline states of polymers., crystalline arrangement of polymers and their morphology.

MODULE - II

Thermodynamics of polymer solutions and their structure determination: Thermodynamics of ideal solutions, regular solutions, lattice model of solutions (Flory – Huggins Theory), Flory – Krigbaum theory for dilute polymer solutions. Fractionation of polymers by different techniques, theory of swelling of cross – linked / network polymers.

Structure determination techniques: X-ray crystallography, NMR, Microscopy: TEM, SEM, STEM, AFM (qualitative treatment only).

MODULE - III

Chain conformation of macromolecules: statistical thermodynamics of interpenetrating random coiling polymers in solution with application to phase separations, swelling of networks, depression of melting point. Methods for molar mass determination by using static methods (osmometry, light scattering, neutron scattering) and by dynamic methods (intrinsic viscosity, size exclusion chromatography, sedimentation).

MODULE – VI

Rheology and Mechanical Properties of Polymers: Brief introduction to rheology and mechanical properties of polymers, phenomena of viscous flow, kinetic theory of rubber elasticity, amorphous polymers and practical importance of their aggregation states, viscoelasticity (experimental and dynamic method). The glassy state and glass transition temperature. Applications of polymers in structural polymers and composites, packaging materials and coatings, transparent and optical materials, biological and medical materials, fluid modifiers and suspension stabilizers.

MODULE – V

Mechanical strength of polymers: Mechanical strength and life time of polymer mechanism of polymer fracture, effect of various factors on the mechanical properties of polymers (effect of size and shape, effect of fillers, effect of cross – linked density).

Polyelectrolytes: The water-soluble charged polymers and their applications. Ionomers (ion containing polymers), conducting polymers, solid polymer electrolytes, mechanism of conductivity. Polymers in combating environmental pollution and as chemical reagents.

Books Recommended:

1. Text Book of Physical Chemistry: G.M. Barrow
2. Text Book of Polymer Chemistry: Billmeyer
3. Polymer Chemistry: P.J. Flory
4. Physical Chemistry of Polymers: A Tagger
5. Physical Chemistry of Macromolecules: C. Tanford
6. Introduction to Polymer Science: V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar
7. Principles of Polymer Science: P. Bhadur and N.V. Sastry

2. Ability Enhancement Courses

SEMESTER-I

L	T	P	Credit
2	0	0	2

MATH-AE-414(A): Mathematics for Chemists

Course Objectives	Prepare students to develop mathematical foundations to understand and create mathematical arguments require in learning many mathematical concepts to be used in Chemistry especially in Physical Chemistry. To motivate students how to solve practical problems using mathematical concepts.
Course Outcomes	: At the end of the course, the students will be able to • Solve the problems based upon Matrices addition, Subtraction and multiplications and to evaluate determinants. • Solve problems based upon differential calculus including Maxima and Minima problems. • Solve the problems based upon integration included double and triple integrations. • Solve the problems based upon differential equations. • Carry out matrix operations, including inverses and determinants.

DETAILED CONTENT

MODULE-I

Vectors: Vectors, dot, cross and triple products etc. gradient, divergence and curl, Vector Calculus.

MODULE-II

Matrix Algebra and its Applications: Definition of matrix, Types of matrices (row, column, null, square, diagonal), Matrix algebra: Addition, subtraction and multiplication by a number, Matrix multiplication, Transpose and adjoint of matrix, Elementary transformation, Representation and applications to solutions of linear equations, Definition of determinant and its properties, Evaluation of determinants.

MODULE-III

Differential Calculus: Functions of single and several variables and their derivatives, Partial derivative of composite function, Total derivative, Maxima and minima theorem.

MODULE-IV

Integral Calculus: General and special methods of integration, Evaluation of definite and some standard integrals. Reduction formulae, applications of integral calculus.

MODULE-V

Differential Equations: Simple differential equations, Separable variables, Homogeneous equations, Exact equations, Linear equations, Equations of first and second order.

Books Suggested:

1. The chemistry Mathematics Book, E.Steiner, Oxford University Press.
2. Mathematical for Physical Chemistry: F. Daniels, Mc. Graw Hill.
3. Applied Mathematics for Physical Chemistry, J.R. Barante, Prentice Hall.
4. Chemical Mathematics D.M. Hirst, Longman

5. The chemistry Mathematics Book, E.Steiner, Oxford University Press.
6. Mathematical for Physical Chemistry: F. Daniels, Mc. Graw Hill.
7. Applied Mathematics for Physical Chemistry, J.R. Barante, Prentice Hall.
8. Chemical Mathematics D.M. Hirst, Longman.

SEMESTER-I

L	T	P	Credit
2	0	0	2

BIOL-AE-414(B): Biology for Chemists

Course Objectives	This paper deals with the basic concepts of biology for those students who were having mathematics in graduation. The present course will help the students to understand the DNA and RNA structural organization and biochemical composition of genetic material; different metabolism reactions in our body and role of ATP as universal energy currency; and general structure of Nucleosides, nucleotides, DNA, RNA structure etc.
Course Outcomes	: The students after the completion of course will be able to • Students will be able to understand the basic principles of biology and biomolecules. • To communicate and interact about the biological principles applied to chemistry.

DETAILED CONTENT

MODULE-I

Cell Structure and Functions: Structure of prokaryotic and eukaryotic cells, intracellular organelles and their functions, comparison of plant and animal cells. Overview of metabolic processes– catabolism and anabolism. ATP– the biological energy currency.

MODULE-II

Carbohydrates: Conformation of monosaccharides, structure and functions of important derivatives of monosaccharides like glycosides, deoxy sugars, myoinositol, amino sugars. Nacetylmuramic acid, sialic acid disaccharides and polysaccharides. Structural polysaccharides cellulose and chitin. Storage polysaccharides-starch and glycogen. Structure and biological function of glucosaminoglycans of mucopolysaccharides.

MODULE-III

Amino-acids, Peptides and Proteins: Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins. Force responsible for holding of secondary structures. α -helix, β -sheets, super secondary structure, triple helix structure of collagen. Tertiary structure of protein-folding and domina structure. Quaternary structure. Amino acid metabolism-degradation and biosynthesis of amino acids, sequence determination: chemical/enzymatic/mass spectral.

MODULE-IV

Lipid: Fatty acids, essential fatty acids, structure and function of triacylglycerols, glycerophospholipids, sphingolipids, cholesterol, bile acids, prostaglandins. Liproproteins-compositiion and function, role in atherosclerosis. Properties of lipid aggregates-micelles, bilayers, liposomes and their possible biological functions. Biological membranes. Lipid metabolism oxidation of fatty acids.

Module-V

Nucleic Acids: Purine and pyrimidine bases of nucleic acids, base pairing via H-bounding. Structure ofribonucleic acids (RNA) and deoxyribonucleic acid (DNA), double helix model of DNA and forces responsible for holding it. Chemical and enzymatic hydrolysis of nucleic acids. The chemical basis for heredity,

an overview of replication of DNA, transcription, translation and genetic code. Chemical synthesis of mono and trinucleoside.

Books Suggested:

1. Principles of Biochemistry, A.L. Lehninger, Worth Publishers.
2. Biochemistry, L. Stryer, W.H. Freeman.
3. Biochemistry, J. David Rawan, Neil Patterson.
4. Biochemistry, Voet and Voet, John Wiley.

SEMESTER-I

L	T	P	Credit
3	0	0	3

CA-AE-415: Computer for Chemists

Course Objectives	The concept of computer basics and programming with particular attention to examples like Fundamentals computational concepts underlying most programming languages and the clear expression of solutions at different levels of abstraction.
Course Outcomes	: The students after the completion of course will be able to • Edit their thesis work confidently. • Calculate complex calculation. • Run differential equation and integration equation programme.

DETAILED CONTENT

MODULE-I

Computer Organization: The evolution of computers, Classification of computers. Block Diagram: Input-output devices, Description of Computer Input Modules, Other Input Methods, and Computer Output Modules. Computer Memory- Memory Cell, Memory Organization, Read Only Memory, Serial Access Memory, Physical Devices Used to construct Memories, Magnetic Hard disk, Compact Disk Read Only Memory, Magnetic Tape Drives.

MODULE-II

Introduction to Computers and Computing: Basic structure and functioning of computers with a PC as an illustrative example. Memory, I/O devices. Secondary storage. Computer languages. Operating systems with DOS as an example. Introduction to UNIX and WINDOWS. Data Processing, principles of programming. Algorithms and flow-charts.

MODULE-III

Computer Programming in C Language: Introduction to C: History and salient features of C, structure of C program, writing and compiling C program, Errors – syntax, semantic, linker, logical and runtime. The C preprocessor, #define, #ifdef, Predefined Names Defined by Preprocessor, Macros Vs Functions.

Variables and Constants: Character Set, Identifiers and Keywords- Rules for Forming Identifiers, Keywords, Data Types and Storage, Data Type Qualifiers, Variables, Declaring Variables, Initializing Variables, Constants-Integer Constants, Floating Point Constants, Character Constants, String Constants, Symbolic Constants

Module-IV

Operators: Operators and Expressions Assignment Statements, Arithmetic Operators, Relational Operators, Logical Operators, Comma and Conditional Operators, Type Cast Operator, Size of Operator, C Shorthand, Priority of Operators

Module-V

Control statements: Decision Control Statements - The if Statement, The switch Statement; Loop Control Statements- The while Loop, The do-while Statement, The for Loop, The Nested Loop; The Goto Statement; The Break Statement; The Continue Statement

Books Suggested:

1. Comdex Computer Course kit (XP Edition), Vikas Gupta, Dreamtech, New Delhi
2. Fox Pro For DOS & Windows, R.K. Taxali, BPB Publication.
3. Programming in ANSIC, E. Balaguruswamy, Tata McGraw Hill
4. Computer for Chemist Bansal, Pragati Prakshan
5. K.V. Raman, Computers in Chemistry, Tata McGraw Hill.
6. Mullish Cooper, The spirit of C, An Introduction to Modern Programming.

SEMESTER-I

L	T	P	Credit
0	0	1	1

CA-AE-419P: Computer Practical

Course Objectives	The objective of this course is to understand the basic knowledge of computer, to gain general awareness of computer software and to understand the automation office.
Course Outcomes	• Should have learnt different variable constructs in programming languages • Should acquire the skill to write programs to solve small problems in chemistry • Ability to apply various computational tools for various applications in chemistry

DETAILED CONTENT

MS Office course trains students how to use MS Office applications use in office work such as creating professional-quality documents; store, organize and analyze information; arithmetic operations and functions; and create dynamic slide presentations with animation, narration, images, and much more, digitally and effectively.

MS word

- Creating, editing, saving and printing text documents
- Font and paragraph formatting
- Simple character formatting
- Inserting tables, smart art, page breaks
- Using lists and styles
- Working with images
- Using Spelling and Grammar check
- Understanding document properties
- Mail Merge

MS Excel

- Spreadsheet basics
- Creating, editing, saving and printing spreadsheets
- Working with functions & formulas
- Modifying worksheets with color & auto formats
- Graphically representing data: Charts & Graphs
- Speeding data entry: Using Data Forms
- Analyzing data: Data Menu, Subtotal, Filtering Data
- Formatting worksheets
- Securing & Protecting spreadsheets

MS Power Point

- Opening, viewing, creating, and printing slides
- Applying auto layouts
- Adding custom animation
- Using slide transitions
- Graphically representing data: Charts & Graphs
- Creating Professional Slide for Presentation.

Internet

- Understanding how to search/Google
- bookmarking and Going to a specific website
- Copy and paste Internet content into your word file and emails
- Understanding social media platforms such as Facebook & Many more
- learn with best practices

Others

Chemdraw, Origin, mathematical equations, etc.

Suggested Readings/ Books:

1. "Computers Today", D. H. Sanders, Fourth Edition, McGraw Hill, 1988.
2. "Fundamentals of Computers", V. Rajaraman, Second Edition, Prentice Hall of India, New Delhi, 1996.
3. "Information Technology", Satish Jain, Paperback Edition, BPB 1999.
4. "Information Technology Inside and Outside", David Cyganski, John A. Orr,Paperback Edition, Pearson Education 2002.
5. "Computer Fundamentals", B. Ram, Third Edition, Wiley, 1997.
6. "Fundamentals of Information Technology", Chetan Srivastva, Third edition, Kalayani Publishers
7. Computers, Larry long & Nancy long, Twelfth edition, Prentice Hall

Open Elective Courses

SEMESTER-II

L	T	P	Credit
2	0	0	2

CHEM-OE-01: Environmental Chemistry

Course Objectives	The specialization in "Environmental Chemistry," will give an insight to the role of various environmentally harmful substances for the degradation of the environment. The students will learn what is toxic, and most importantly, will become an expert on what we can do to find solutions to the challenges of toxic substances in the environment.
Course Outcomes	At the end of the course, the student will be able to • Acquire fundamental knowledge and understanding of the physical environment (land, water, air and climate) and will develop insights into key concepts in the field of environmental Chemistry. • Understand the basic phenomena of atmospheric sciences, hydrology of different aquatic ecosystems and soil science. • Develop sound theoretical background of basic chemistry associated with toxicology of environmental pollutants • Get acquainted with the sources, properties and ill-effects of important air, water, soil and radioactive pollutants in air, water and soil and apply analytical tools to determine and measure pollutants in various environmental samples • Become aware of the local, regional and global environmental problems.

DETAILED CONTENT

MODULE-I

Environmental Chemistry: Atmosphere, environmental segments, composition of the atmosphere, earth's radiation balance, particulates, ions and radicals and their formation, chemical and photochemical reactions in the atmosphere, air pollution, oxides of C,N,S and their effects, acid-rain, smog formation, Green house effects (global warming and ozone depletion, air pollution controls and introduction to analytical methods for monitoring air pollution.

MODULE-II

Hydrosphere: Chemical composition of water bodies-lakes, streams, rivers, sea etc, hydrological cycle, complexation in natural and waste water and microbially mediated redox reactions. Water pollution-inorganic, organic, pesticides, industrial and radioactive materials, oil spills and oil pollutants, eutrophication, acid-mine drainage, waste water treatment, domestic waste water (aerobic and anaerobic treatment), and industrial waste water treatment.

MODULE-III

Water quality parameters and standards: Analytical methods for measuring DO, BOD, COD, fluoride, oils and grease and metals (As, Cd, Hg, Pb, Zn, Cu, Cr).

Lithosphere: Soil composition, micro and macro nutrients, soil pollution- fertilizers, pesticides, As, Cd, Hg, Pb, Cr, and CN, etc.

Books recommended:

1. *Principles of Biochemistry -A.L.Lehringer*
2. *Introduction to Chemistry of Life-H.J.DeBay*
3. *Outlines of Biochemistry-Conn and Stumpf*
4. *Environmental Chemistry-A.K.De*
5. *Environmental Chemistry-Manaham*
6. *Environmental Pollution Analysis-Khopkar*

SEMESTER-III

L	T	P	Credit
2	0	0	2

CHEM-OE-02: Chemistry in Daily Life

Course Objectives	The course will focus on the role of chemistry in necessities of daily life such as food, beverages, housing, healthcare, and development of biodegradable polymers. In addition it will introduce various applications of chemistry in the area of medical, dairy, corrosion and polymer industries.
Course Outcomes	• This course will help students in solving many future problems, including sustainable polymers in medical and aerospace field, managing our environment, providing safe drinking beverages or foods and promoting human and environmental health.

DETAILED CONTENT

MODULE-I

Dairy Products: Composition of milk and milk products. Analysis of fat content, minerals in milk and butter. Estimation of added water in milk. Beverages: Analysis of caffeine in coffee and tea, detection of chicory in coffee, estimation of methyl alcohol in alcoholic beverages.
Food additives, adulterants and contaminants- Food preservatives like benzoates, propionates, sorbates, disulphites. Artificial sweeteners: Aspartame, saccharin, dulcin, sucralose and sodium cyclamate. Flavours: Vanillin, alkyl esters (fruit flavours) and monosodium glutamate. Analysis of pesticide residues in food.
Artificial food colorants: Coal tar dyes and non-permitted colours and metallic salts.

MODULE-II
Vitamins: Classification and Nomenclature. Sources, deficiency, diseases and structures of Vitamin A1, Vitamin B1, Vitamin C, Vitamin D, Vitamin E & Vitamin K1.
Oils and fats: Composition of edible oils, detection of purity, rancidity of fats and oil. Tests for adulterants like argemone oil and mineral oils.
Soaps & Detergents: Definition, classification composition and uses

MODULE-III

Corrosion: Types and prevention, corrosion failure and analysis Chemical energy system and limitations.
Fuel Cells: Principles and applications of primary & secondary batteries and fuel cell. Basics of solar energy, future energy storer**.**

Polymers: Types and classification of polymers. Source and general characteristics of natural and synthetic polymers. Typical examples of polymers used as plastics, in textiles, in electronic and automobile components, in

the medical and aerospace materials. Problems of plastic waste management. Strategies for the development of environment friendly polymers.

Books recommended:

1. B. K. Sharma: introduction to Industiral Chemistry, Goel Publishing, Meerut (1998)
2. Medicinal Chemistry by Ashtoush Kar.
3. Drugs and Pharamaceutical Sciences Series, Marcel Dekker, Vol. II, INC, New York
4. Analysis of Foods – H.E. Cox: 13. Chemical Analysis of Foods – H.E.Cox and pearson.
5. Foods: Facts and Principles. N. Shakuntala Many and S. Swamy, 4th ed. New Age International (1998) 6. Physical Chemistry – P l Atkins and J. de Paula – 7 th Ed. 2002, Oxford University Press.
7. Handbook on Feritilizer Technology by Swaminathan and Goswamy, 6th ed. 2001, FAI.
8. Organic Chemistry by I. L. Finar, Vol. 1 & 2. 9. Polymer Science and Technology, J. R. Fired (Prentice Hall).