Sardar Patel University Mandi

District Mandi -175001 (HP) India

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(Established Under H.P. Legislative Assembly Act 03 of 2022)

Syllabus for M.Sc. Chemistry

2 Years (CBCS)

Session 2022-23 Onwards

Faculty of Physical Sciences

Sardar Patel University Mandi (HP)

HIMACHAL PRADESH UNIVERSITY
DEPARTMENT OF CHEMISTRY

PROCEEDINGS OF THE MEETING OF THE BOARD OF STUDIEIS IN (PG) IN THE SUBJECT OF CHEMISTRY

A meeting of the Board of Studies in PG in the subject of Chemistry was held on 24.12.2021 at 2.00PM in the Departmental Library of the Chemistry Department. The following were present:

1	Prof. Baljit Singh	Chairman & Convener
2	Prof. Suman Lata Department of Chemistry, Deenbandu Chhotu Ram University of Science and Technology, Muruthal, Haryana.	External Expert
3	Prof. Gurjaspreet Singh, Department of Chemistry, Punjab University Chandigarh.	External Expert (attended online meeting)
4	Prof. Suvarcha Chauhan	Member
5	Dr. Sandeep Chauhan	Member
6	Dr. Kiran Kumar	Member
7	Dr. Rajesh Kumar	Member

The following decisions were taken:

1. The scheme as well as the course contents of the syllabi of M. Sc. Chemistry (CBCS), spread over four semesters (I-IV) applicable w. e. f. the Academic Session 2022-2023 i.e. July, 2022 onwards, was discussed and recommended for the consideration of the Faculty of Physical Sciences (as per annexure "A") .

2. In order to maintain the academic standard in respect of research and teaching and also to maintain the uniformity in PG courses offered by HP University to the affiliated institutes (both private and Govt. colleges), the BOS recommended that the all the affiliated institutes will conduct the P.G. practical examinations by the panel of examiners recommended by the chairman of the BOS with subsequent approval of the competent authorities of the University. The practical examination conducted without approved panel of the examiner will not be considered valid for M.Sc. Chemistry degree.

3 The BOS authorized the Chairman & Convener of the BOS (PG) to make typographic corrections and mistakes if any.

4. It was resolved by the BOS (PG) that the pass percentage will be 40% for the M. Sc (Chemistry) . The detail of pass percentage will be as under:

A. In Theory - 40% (32/80)
B. In I.A. - 40% (08/20)
C. In Practical - 40% (20/50)

The meeting ended with a vote of thanks to the chair.

Prof. Suman Lata
External Expert

Prof. Gurjaspreet Singh
External Expert

Prof. Suvarcha Chauhan
Member

Dr. Sandeep Chauhan
Member

Dr. Kiran Kumar
Member

Dr. Rajesh Kumar
Member

Prof. Baljit Singh
Chairman & Convener

Annexure-"A"

A Detailed Scheme and Course Contents of the Syllabi for M.Sc. Chemistry Spread Over Four Semesters (I-IV) For Session 2022-23 and Onwards

Course number	Course Title	Course Type	Credits	Teaching Hours per week	Maximum marks theory + Internal assessment =Total Marks
		Semester I			
CHEM 101	Inorganic Chemistry Theory -1	CP	4	4	80+20=100
CHEM 102	Organic Chemistry Theory -1	CP	4	4	80+20=100
CHEM 103	Physical Chemistry Theory -1	CP	4	4	80+20=100
CHEM 104	Mathematics for Chemists	GE	3	3	40+10=50
CHEM 105	Applications of computer in Chemistry	SEC	3	3	40+10=50
CHEM 106	Inorganic Chemistry Practical -1	CP	3	6	50
CHEM 107	Organic Chemistry Practical -1	CP	3	6	50
CHEM 108	Physical Chemistry Practical -1	CP	3	6	50
Total			**27**		**550**
		Semester II			
CHEM 201	Inorganic Chemistry Theory -2	CP	4	4	80+20=100
CHEM 202	Organic Chemistry Theory -2	CP	4	4	80+20=100
CHEM 203	Physical Chemistry Theory -2	CP	4	4	80+20=100
CHEM 204	Chemistry of Life Science	GE	3	3	40+10=50
CHEM 205	Environmental Chemistry	GE	3	3	40+10=50
CHEM 206	Inorganic Chemistry Practical -2	CP	3	6	50
CHEM 207	Organic Chemistry Practical -2	CP	3	6	50
CHEM 208	Physical Chemistry Practical -2	CP	3	6	50
Total			**27**		**550**
		Semester III			
CHEM 301	Inorganic Chemistry Theory -3	CP	4	4	80+20=100
CHEM 302	Organic Chemistry Theory -3	CP	4	4	80+20=100
CHEM 303	Physical Chemistry Theory -3	CP	4	4	80+20=100
CHEM 304	Inorganic Chemistry Special Theory -1	DSE	4	4	80+20=100
CHEM 305	Organic Chemistry Special Theory -1	DSE	4	4	80+20=100
CHEM 306	Physical Chemistry Special Theory -1	DSE	4	4	80+20=100
CHEM 307	Inorganic Chemistry Practical -3	CP	3	6	50
CHEM 308	Organic Chemistry Practical -3	CP	3	6	50
CHEM 309	Physical Chemistry Practical -3	CP	3	6	50
Total			**25**		**550**
	Candidate will choose only one specialization in Semester III & Semester IV				
		Semester IV			
CHEM 401	Inorganic Chemistry Special Theory -2 (Advanced Organometallic)s	DSE	4	4	80+20=100
CHEM 402	Inorganic Chemistry Special Theory -3 (Modern Techniques of Chemical Analysis)	DSE	4	4	80+20=100
CHEM 403	Inorganic Chemistry Special Theory -4 (Inorganic Spectroscopy)	DSE	4	4	80+20=100
CHEM 404	Inorganic Chemistry Special Theory -5 (Bio-Inorganic Chemistry)	DSE	4	4	80+20=100
CHEM 405	Organic Chemistry Special Theory -2 (Organic Synthesis)	DSE	4	4	80+20=100
CHEM 406	Organic Chemistry Special Theory -3 (Natural products)	DSE	4	4	80+20=100
CHEM 407	Organic Chemistry Special Theory -4 (Medicinal Chemistry)	DSE	4	4	80+20=100
CHEM 408	Organic Chemistry Special Theory -5 (Polymer Chemistry)	DSE	4	4	80+20=100
CHEM 409	Physical Chemistry Special Theory -2 (Advanced Quantum Chemistry)	DSE	4	4	80+20=100
CHEM 410	Physical Chemistry Special Theory -3 (Solid State Chemistry)	DSE	4	4	80+20=100
CHEM 411	Physical Chemistry Special Theory -4 (Biophysical Chemistry)	DSE	4	4	80+20=100
CHEM 412	Physical Chemistry Special Theory -5 (Chemistry of Macromolecules)	DSE	4	4	80+20=100
CHEM 413	Inorganic Chemistry Special Practical -1	DSE	6	8	100
CHEM 414	Organic Chemistry Special Practical-1	DSE	6	8	100
CHEM 415	Physical Chemistry Special Practical-1	DSE	6	8	100
CHEM 416	Two Seminar*	AEC	4	8	50 (Single award list) [25] x 2 =50
Total			**26**		**550**
For practical examination, single award list will be prepared which includes marks of practical and internal assessment of practical (20%) for each practical course.					

[1] The abbreviations use in the above course types are as follows:

Core papers = CP
Discipline Specific Elective= DSE
Generic Elective = GE
Ability Enhancement Courses= AEC
Skill Enhancement Courses =SEC

[2] Students will opt DSE course as per their specialization i.e. Inorganic, Organic and Physical chemistry.

[3] The examination time for each theory paper will be of three hours.

[4] The examination time for practicals of first, second and third semester will be of 6 hrs in two sessions (i.e. both morning and evening).

[5] The examination time for practical's of fourth semester will be of 12 hrs in four sessions (i.e. in two days both morning and evening)

[6] For Internal Assessment (I.A.), the following criteria will be implemented with regards to the award of internal assessment:

i) Internal Assessment (I.A.) of 20 % Marks will be added to each paper.
ii) These marks would , however be split as following: (a) 5 Marks for attendance in theory as well as in practical classes. The Weightage to attendance will be as follows: upto 75% with condonation from competent authority as per provision under ordinance-ZERO. Without condonation upto 75%- ONE MARK. 76-80%- TWO MARKS, 81-85% THREE MARKS, 86-90%- FOUR MARKS and above 91% FIVE MARKS.
iii) The award of 15 Marks would be based on the performance of one class test of 15 Marks and this Test will consist of both subjective as well as objective type questions.

[7] Total Marks of all Four Semesters

Semester	**Credits**	**Marks**
Semester I	27	550
Semester II	27	550
Semester III	25	550
Semester IV	26	550
Grand Total	105	2200

SEMESTER-I
CHEM 101
Inorganic Chemistry Theory -1

Lectures-60
Max. Marks-80

Course Objectives: This is an introductory inorganic chemistry course which will help in thoroughly understanding the concepts and the applications of group theory, non aqueous solvents, clusters, supramolecular chemistry and consequently in development of the aptitude for academic and professional skills.

Note: i. *Ten questions will be set by the examiner selecting* ***TWO*** *from each unit. As far as possible every question will be divided into* ***Two – Three Parts****. The students shall attempt* ***FIVE*** *questions selecting* ***ONE*** *from each unit .****ii.*** *Students can ask for Character Tables (except for C2V and C3V point groups) if required.*

UNIT-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.

UNIT-II
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 a dehydrating agent, as an oxidizing agent, as a medium to carry out acid-base neutralization reaction and as a differentiating solvent. Liquid BrF3: Physical properties, solubilities in BrF3, self-ionization, acid base neutralization reactions, solvolytic reactions and formation of transition metal fluorides.

UNIT-III
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) and carboranes,

UNIT-IV
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 the following reagents in analysis:
(a) Dimethylglyoxime (in analytical chemistry)
(b) EDTA (in analytical chemistry and chemotherapy)
(c) 8-Hydroxyquinoline (in analytical chemistry and chemotherapy)
(d) 1,10-Phenanthroline (in analytical chemistry and chemotherapy)
(e) Thiosemicarbazones (in analytical chemistry and chemotherapy)
(f) Dithiazone (in analytical chemistry and chemotherapy)

UNIT-V
Supramolecular Chemistry (Ref. Book 15): 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)

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,VthEdn.
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
15. Supramolecular Chemistry (Concepts and Perspectives) - Jean Marie Lehn(VCH-1995).

Course Outcomes:
CO 1: Apply the concepts of symmetry operation, character tables, group representation to describe the geometries and chemical bonding of molecules
CO2: Explain the chemistry and mechanisms of transition metal fluorides in the presence of non-aqueous solvents.
CO 3: Classify the various kind of metal clusters with reference the metal boranes and carboranes
CO 4: Understand and describe the role of some organic reagents in inorganic chemistry.
CO 5: Know the basic concepts associated with supramolecular chemistry and their applications.

SEMESTER-I
CHEM 102
Organic Chemistry Theory -1

Lectures: 60
Max. Marks: 80

Course Objectives : The main objective of this course is to provide basic to advance level of knowledge to the students regarding supramolecular chemistry, stereochemistry and reaction mechanism. To develop a basic understanding about the structure and reactivity relationship. To understand mechanistic details of different types of aliphatic nucleophilic substitution, aliphatic electrophilic substitution and free radical reactions.

Note: *Ten questions will be set by the examiner selecting **TWO** from each unit. As far as possible every question will be divided into **Two – Three Parts**. The students shall attempt **FIVE** questions selecting **ONE** from each unit.*

UNIT I
Supramolecular Chemistry: Introduction, Bonding other than covalent bond. Addition compounds, Crown ether complexes and Cryptands, Inclusion compounds, Cyclodextrins, Catenanes and Rotaxenes and their applications.

UNIT II
Stereochemistry: Introduction to Basic Concepts of Stereochemistry: Isomers and their properties, Threo and Erythro isomers, Chirality, Optical isomerism, Geometrical isomerism, Conventions for configurations- D,L and R,S systems, Racemic mixture and Racimization, Resolution of Racemic mixtures, Measurement of optical activity, optical purity, Streoselective and Streospecific reactions, epimerization, epimers, anomers and mutarotation, Axial Chirality (Allenes and Biphenyls), Planar chirality, Helicity, Chirality involving atoms other than carbon atoms, Prochirality: prostreoisomerism and Asymmetric synthesis.
Conformational and streoisomerism of acylic and cylic systems, cyclohexane, decalins, effect of conformation on reactivity in acylic and cyclohexane systems.

UNIT 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 mechanisms,

UNIT IV
Aliphatic Nucleophilic Substitution: Reactivity effect of substrate structure, leaving group and nucleophile. 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, Phase-transfer catalysis, and ultrasound, ambident nucleophile, regioselectivity.

UNIT V
Aliphatic Electrophilic substitution: Bimolecular mechanisms- SE_2 and SE_i. The SE_1 mechanism, electrophilic substitution accompanied by double bond shifts, halogenation 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 alkanes, Stork-enamine reactions.
Free radical reactions: Geometry of free radicals, 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), 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.

Course Outcomes:
CO1: Know about the supramolecular chemistry and bonding to explain its various applications.
CO2: Apply the basic concepts of stereochemistry and various types of stereoisomers of organic molecules to understand the effect of conformation on reactivity of organic molecules.
CO3: Compare the Kinetic and Thermodynamic requirements of the reactions to establish mechanism of organic reaction.
CO4: Analyze the mechanistic details of different types of aliphatic nucleophilic substitution reactions.
CO5: Apply the mechanistic details of different types of aliphatic electrophilic substitution and free radical reactions.

SEMESTER-I
CHEM 103
Physical Chemistry Theory -1

Lectures: 60
Max. Marks: 80

COURSE OBJECRTIVES: This course is introduced to impart students with the knowledge of various spectroscopic techniques viz; NMR, ESR, Mossbaur and molecular spectroscopy along with kinetics of various complex and fast reactions and catalytic activity at surfaces.

Note: *Ten questions will be set by the examiner selecting* ***TWO*** *from each unit. As far as possible every question will be divided into* ***Two – Three Parts****. The students shall attempt* ***FIVE*** *questions selecting* ***ONE*** *from each unit.*

UNIT – I
Resonance Spectroscopy: Principle and Theory of nuclear magnetic resonance (NMR). Chemical shift and spin – spin coupling. Factors influencing chemical – shift and spin – spin coupling of ^{1}H-NMR. Spin – spin and spin – lattice relaxation processes. Line –width and rate processes. First and second order ^{1}H-NMR spectra. Principle and theory of Electron Spin Resonance (ESR). Hyperfine structure of ESR. Zero – field splitting of ESR signal., McConnell relation.Introduction to Mossbaur spectroscopy (isomer – shift, quadrupole interaction and magnetic hyperfine interaction).

UNIT - II
Molecular Spectroscopy: Rotational spectra of non – rigid diatomic molecules and symmetric - top molecules. Anharmonic oscillator, overtones and hot bands. Diatomic vibrator – rotator (P, Q and R – branches). Rotational – vibrational spectra of symmetric – top molecules. Raman Spectroscopy. Rotational and vibrational Raman spectra of linear and symmetric top molecules, overtones and mutual exclusion principle.

UNIT - III
Kinetics of complex reactions: Consecutive and competitive (parallel) first order reactions. Kinetic vs. thermodynamic control reaction. Free radical reactions; 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 or ½ order reactions. Reaction rates and chemical equilibrium, principle of microscopic reversibility, activation energy and activated complex.

UNIT - IV
Transition state theory and its kinetic and thermodynamic formulation. Introduction to Potential energy surfaces. Kinetics in solutions: diffusion controlled reactions, their rates and influence of the solvent. Collisions and transition state theories in simple gas reactions, Lindman and Hinshelwood treatment.

UNIT - V
Catalytic activity at surfaces: adsorption and catalysis, the Langmuir – Hinshelwood mechanism, the Eley – Rideal mechanism. Examples of catalysis: hydrogenation, oxidation and cracking and reforming (qualitative treatment only). Introduction to fast reactions. Flash photolysis and Stopped flow methods to study the kinetics of 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 Reaction:C. Kalidas
7. Fast Reactions in Solutions: Caldin
8. Basic Principles of Spectroscopy: R. Chang
9. NMR and Chemistry: J.W. Akit
10. Introduction to Molecular Spectroscopy: G.M. Barrow
11. Physical Chemistry: P.W. Atkins
12. Fundamentals of Molecular Spectroscopy: C.N. Banwell
13. Physical Chemistry: G.K. Vemulapalli

Course Outcomes:
CO1: Explain principles of various spectroscopic techniques
CO2:Interpret and analyse spectra of the molecules using rules of various spectroscopic techniques
CO3: Solve problems by choosing suitable spectroscopic methods and interpreting corresponding data
CO4: Understand the mechanisms and kinetics of complex and fast reactions
CO5: Explain the function and purpose of a catalyst and mechanisms involved in catalysis.

SEMESTER-I
CHEM 104
Mathematics for Chemists

Lectures: 48
Max. Marks: 40

Objective of the course: To impart the basic knowledge of mathematical tools needed to solve the chemistry problems.

Note: *Ten questions will be set by the examiner selecting* ***TWO*** *from each unit. As far as possible every question will be subdivided into* ***Two – Three Parts****. The students shall attempt* ***FIVE*** *questions selecting* ***ONE*** *from each unit.*

UNIT - I

Differential calculus: Idea of functions, Limit and Continuity, functions of single and several variables, derivatives, partial derivatives, total derivative. Graphical representation of differentiation, Rules of Differentiation, maxima and minima.

Some examples related to chemistry: (i) Calculation of the rate of change of λ with θ in Bragg equation, (ii) Calculation of equilibrium separation between two helium atoms separated by a distance R in the Lennard-Jones potential V, (iii) Calculation of $\left(\frac{\partial V}{\partial T}\right)_p$, $\left(\frac{\partial T}{\partial p}\right)_V$ from the ideal gas equation, (iv) Calculation of $\left(\frac{d}{dv}\right)f(v)$ for The Maxwell Boltzmann Distribution $f(v) = Av^2e^{-Bv^2}$ of molecular velocities, (v) Calculation of $\left(\frac{dp}{d\zeta}\right)$ for the reaction $N_2O_4 \rightleftharpoons 2\ NO_2$, where $p(N_2O_4) = \frac{1-\zeta}{1+\zeta}$

UNIT – II

Integral calculus: Methods of integration, geometric interpretation of integral, evaluation of some simple definite integrals. Significance of 'exponential' equations. Some integrals related to chemistry:

(i) The significance of 'exponential' equations, (ii) Calculation of work done on an ideal gas compressed isothermally using relation $= -\int_{V_1}^{V_2} PdV$, (iii) Rate expressions for Zero and First order

UNIT-III

Differential equations: Types and classification of differential equations, homogeneous differential equations, exact differential equations, linear equations, and differential equations of first and second orders, Solution of first order differential equations.

Application to simple chemistry problems: Solving Particle in one dimensional box by taking (a) trigonometric functions (b) exponential functions.

UNIT – IV

Matrices and Determinants: Definition of matrix, types of matrices (row, column, null, square, diagonal).

Matrix algebra: Multiplying a matrix by a constant, addition, subtraction and multiplication of two matrices. Transpose and adjoint of a matrix, elementary transformation, representation and applications to solutions of linear equations.

Application of Matrices to simple chemistry problems: (i) Finding the atom connectivity matrix for molecules like but-1-ene (hydrogens ignored), (ii) Writing Huckel Molecular Orbital secular equations for 1,3 butadiene, cyclobutadiene, benzene, water, Ammonia.

UNIT-V

Vectors: representation and simple properties of vectors, addition and subtraction of vectors, addition by the method of triangles, resolution of vectors. Scalar product of vectors. Concept of normalization, orthogonality and complete set of unit vectors. Application to simple chemistry problems:(i) Calculation of speed of particle moving with velocity ($\vec{v}$) in two-dimensional space, three-dimensional space, (ii) calculation of work done (w) by the vector force on a particle of velocity ($\vec{v}$) in the given time interval using $W = \int_{t_1}^{t_2} F.v\ dt$.

Suggested Books:

1. Maths for Chemists, Allan Cunningham, RoryWhelan, University of Birmingham University of Leeds, available online;
   https://www.birmingham.ac.uk/Documents/college-eps/college/stem/Student-Summer-Education-Internships/Maths-for-Chemists-Booklet.pdf
2. Mathematical Preparation for Physical Chemistry, F. Daniels, McGraw Hill.
3. Mathematical Preparation for General Physics, J.B. Marian, R.C. Davidson Saunder Company.
4. Mathematical Methods for Science Students, G. Stephemen, ELBS.
5. Applied Mathematics for Physical Chemistry: T.R. Barrante
6. Chemical Thermodynamics, C.E. Reid, Mc Graw Hills, College 0^{th} Edition.

Course outcomes:

CO1:Apply basic knowledge of Differential calculus for the use of chemists.

CO2:Apply the general methods of integration for their application to solve chemistry problems.

CO3: Apply basic knowledge of differential equations used in chemistry.

CO4: Apply basic knowledge of Matrices and Determinants to solve chemistry problems.

CO5: Apply basic knowledge of Vectors to evaluate physical parameters related to chemistry.

SEMESTER-I
CHEM 105
APPLICATION OF COMPUTER IN CHEMISTRY

Lectures: 48
Max. Marks: 40

Objectives of the course: To impart basic knowledge of computers to chemistry students and to acquaint them to use tools of computers to solve chemistry problems.

Note: *Ten questions will be set by the examiner selecting* ***TWO*** *from each unit. As far as possible every question will be subdivided into* ***Two – Three Parts****. The students shall attempt* ***FIVE*** *questions selecting* ***ONE*** *from each unit.*

UNIT – I

Introduction: Characteristics of Computer, Evolution of computer, Capabilities and limitations of computer, Generations of computer, Types of computers (micro, mini, main frame, supercomputers), Block diagram of computer, Basic components of a computer system, Input unit, Output unit, Arithmetic logic Unit, Control unit and Central Processing Unit.

UNIT – II

Computer Software: Software and its Need, Types of softwares, System software, Application software, operating system, utility program, programming languages, introduction to operation system for PCs-DOS, windows, linux, application software and its types – word processing, spreadsheet, presentation and graphics.

UNIT – III

Internet Concepts: Basics of Networking – LAN, WAN, Wi-Fi technologies and sharing of printers and other resources, Concept of IP addresses, applications of internet like: e-mail and browsing, concept of search engine and safe searching. Various browsers like Internet explorer/Microsoft Edge, Mozilla Firefox, use of cookies and history, WWW (World Wide Web), hyperlinks and introduction to Anti-virus.

UNIT – IV

Chemistry and FORTRAN Programming: Introductory FORTRAN concepts, character set, constant variables, data types, subscripted variables, and FORTRAN functions.
Data transfer and program execution control: Introduction, format specification for READ and WRITE statements, format commands, control commands and transfer commands. Logical variable and Double precision variables

UNIT – V

Arrays and repetitive computation: Introduction, arrays arrange storage, dimension statement, do continue, Nested do – loop continue statement, implied do. Sub – programme (functions and sub –routines): COMMON and DATA statements. Sub programme, function arguments, subroutines, save variable function vs. subroutine programme.

Books Recommended:

1. Hunt, R.; Shelley, J. Computers and Common Sense, Prentice Hall.
2. Norris, A.C. Computational Chemistry, 1st edition, John Wiley & Sons, 1981.
3. Rajaraman, V. Computer Programming in FORTRAN IV, 4th edition, Prentice Hall India Pvt. Ltd., 1997.
4. Rajaraman, V.; RadhaKrishnan, V. An Introduction to Digital Computer Design, Prentice Hall.
5. Fortran 77 & 90: V. Rajaraman
6. Computer in Chemistry: K.V. Raman
7. Microcomputer Quantum Mechanics, Second Edition; J.P. Killingback and Adam Hilger Ltd., Bristol and Boston, 1985.
8. quick basic Programming for Scientists and Engineers; Joseph H. Noggle; CRC Press, 1992.
9. Meth Norton's; Introduction to Computers; Fourth Edition; McGraw Hill, New York.
10. Computers for Chemists; K.V. Rajoraman; Tata Megraw Hill Co. Ltd.; New Delhi; 1993.

Course outcomes:

CO1: Develop basic knowledge of computers.
CO2: Develop basic knowledge of computer hardware.
CO3: Develop basic knowledge of computer software.
CO4: Explain the functions in FORTRAN for data analysis in chemistry.
CO5: Use of functions in FORTRAN for chemistry applications.

SEMESTER I
CHEM 106
Inorganic Chemistry Practical -1

Time - 6 hr/week
Max. Marks – 50

Course Objectives: The Course is introduced to impart practical knowledge of the chemical methods of analysis with basic titrimetric and gravimetric techniques to students. It will enable the students to develop their experimental skills and creativity.

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) 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 damasking agents
- v) Determination of hardness of water

Books Recommended:

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

Course Outcomes:

CO 1: Know the various types of titrimetric methods of analysis and their applications.
CO 2: Demonstrate the iodatometric, bromatometric cerimetric and acid base and complexometric titrations in laboratory.
CO 3: Perform experimentation and evaluate the results.
CO 4: Develop the ability to compile interpreted information in the form of lab record and to face viva-voce

SEMESTER I
CHEM 107
Organic Chemistry Practical -1

Time : 6 hr/week
Max. Marks : 50

Course Objectives: The objective of this course is to provide basic knowledge to students regarding laboratory & purification techniques in organic chemistry. To know the concept of stepwise synthesis of the organic compounds and to know the practical applicability of different types of organic reactions.

Demonstrations of Laboratory & Purification techniques: Refluxing, Solvent extraction, Purification of solvents and reagents using various techniques like crystallization, distillation, steam distillation, vacuum distillation. Drying and storage of solvents, sublimation etc.
Preparation of some important organic compounds involving the reactions out of the followings representative reactions Acetylation, Esterification, Oxidation, Reduction, Nucleophilic substitution, Aromatic electrophilic substitution reaction, Condensation reactions, Hoffman's Bromamide reaction.
Oxidation: Adipic acid by chromic acid oxidation of cyclohexanol , Grignard reaction: Synthesis of triphenyl methanol from benzoic acid. Sandmeyer reaction: p-chlorotoluene from p-toluidine, Aldol condensation: Dibenzal acetone from benzaldehyde. Acetoacetic ester condensation: Synthesis of ethyl-n-butylacetoacetate, Preparation of iodoform from acetone (Haloform reaction). Preparation of polystyrene, anthranilic acid, fluoresceine-eosin, and methyl orange dyes, and any other reaction as per requirement.
All the students must submit the recrystallised product along with yield, and melting point for all the stages of preparation.

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.

Course Outcomes:
CO1: Describe and demonstrate the basic principle and techniques of purifications.
CO2: Know the concept of stepwise synthesis of the organic compounds.
CO3: Develop the skill of performing experiments and analysing data to evaluate results.
CO4: Develop the ability to compile interpreted information in the form of lab record.
CO5: Learn to face the viva-voce examinations.

<u>SEMESTER I</u>
CHEM 108
Physical Chemistry Practical -1

Time - 6 hr/week
Max. Marks - 50

Course objectives: This course is introduced to impart knowledge and understanding of various methods used for the determination of refractive index, surface tension and viscosity of various solvents and mixtures along with various experimental methods to analyse the kinetics of various reactions

1. **Refractive Index (RI) Measurements:** Refractive index measurements of pure solvents and analysis of solvent mixtures in terms of composition from the calibration plot.

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

3. **Viscosity Measurements:** Determination of relative and absolute viscosity of the given solvent, determination of percentage composition of a liquid, determination of molar mass of a polymer.

4. **Chemical Kinetics:** Comparison of strengths of two acids by kinetic study, determination of temperature coefficient of a reaction rate, acid hydrolysis of ethylacetate and Saponification of ethylacetate

Books Recommended:

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

COURSE OUTCOMES:
CO1: Understand the safe handling of chemicals, environmental issues, and safety measures to be followed during the labs
CO2: Use various methods in determining the refractive index of various solvents and mixtures
CO3: Determine surface tension and viscosity of various solvents and mixtures by using different experimental methods
CO4: Analyse the mechanisms and kinetics of various reactions by using different experimental methods

SEMESTER-II
CHEM 201
Inorganic Chemistry Theory -2

Lectures-60
Max. Marks-80

Course Objectives: To introduce the fundamental concepts of metal ligand bonding and atomic spectroscopy helpful in interpreting the electronic spectra of metal complexes and their magnatochemistry. To enable understanding of various electronic and magnetic properties of metal complexes helpful in the synthesis of new metal complexes leading to the development of advanced inorganic chemistry.

Note: *Ten questions will be set by the examiner selecting* ***TWO*** *from each unit. As far as possible every question will be divided into* ***Two – Three Parts****. The students shall attempt* ***FIVE*** *questions selecting* ***ONE*** *from each unit.*

UNIT-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)

UNIT-II
Atomic Spectroscopy: Energy levels in an atom, coupling of orbital angular momenta, coupling of spin angular momenta, spin orbit coupling, spin orbit coupling *p2* 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 *d2* configuration), Calculation of the number of the microstates.

UNIT-III
Electronic Spectra-I: Splitting of spectroscopic terms (S,P,D.F and G,H,I), d^{11}-d^9 systems in weak fields (excluding mathematics), strong field configurations, transitions from weak to strong crystal fields.

UNIT-IV
Electronic Spectra-II: Correlation diagrams (d^{11}-d^9) in Oh and Td environments, spin-cross over in coordination compounds. Tanabe Sugano diagrams, Orgel diagrams, evaluation of B,C and β parameters.

UNIT-V
Magnetochemistry: Origin of Magnetic moment, Magnetic susceptibility (diamagnetic, paramagnetic), spin only moment, Russell Saunder's coupling, quenching of orbital angular moment, orbital contribution to a magnetic moment, magnetic moments from magnetic susceptibilities, temperature dependence of magnetic susceptibility, Factors determining paramagnetism, application of magnetochemistry in co-ordination chemistry in spin free and spin paired octahedral and tetrahedral complexes, Van Vlecks formula for 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. Introduction to Magnetochemistry – A.Earnshaw, Academic Press.

Course Outcomes:
CO 1: Explain the crystal field theory and apply the concept of molecular orbital theory to explain stability of coordination complexes.
CO 2: Apply the basic principles of the atomic spectroscopy to identify the energy levels of the atoms, to calculate the number of microstates.
CO 3: Understand the splitting of spectroscopic terms in coordination compounds under applied magnetic field.
CO 4: Interpret the correlation diagrams in octahedral and tetrahedral transition metal complexes.
CO 5:Analyze the magnetic properties of co-ordination compound by applying the basic concepts of magneto-chemistry.

SEMESTER-II
CHEM 202
Organic Chemistry Theory -2

Lectures: 60
Max. Marks: 80

Course Objectives: To understand mechanistic details of different types of aromatic electrophilic substitution, aromatic nucleophilic substitution, elimination and pericyclic reactions. As part of this course, students will be introduced to some reagents used in organic synthesis. To know about some common organic reactions and their mechanisms.

Note: *Ten questions will be set by the examiner selecting* ***TWO*** *from each unit. As far as possible every question will be divided into* ***Two – Three Parts****. The students shall attempt* ***FIVE*** *questions selecting* ***ONE*** *from each unit.*

UNIT -I
(A) Aromatic Electrophilic Substitution: Arenium ion mechanism, orientation and reactivity, The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles, Diazonium coupling, Vilsmeir - Haack reaction, Scholl reaction, Amination reaction, Fries rearrangement, Hofmann-Martius Reaction, Reversal of Friedel Craft alkylation.
(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.

UNIT -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.

UNIT -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.

UNIT -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. Mechanism and Orientation in Pyrolytic eliminations, Cis elimination, elimination in cyclic systems, eclipsing effects, cleavage of quaternary ammonium hydroxides, Shapiro reaction, Conversion of Ketoxime to nitriles.

UNIT -V
Pericyclic Reactions: 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.

Course Outcomes:
CO1: Apply the concept of aromatic electrophilic and nucleophilic substitution reactions to explain their applications.
CO2: Explain the synthesis and applications of some reagents used in organic synthesis.
CO3: Know about some common organic reactions and to explain their mechanisms.
CO4: Understand the mechanistic implications of Elimination Reactions
CO5: Analyze the concept of molecular orbital symmetry to apply in pericyclic reactions.

SEMESTER-II
CHEM 203
Physical Chemistry Theory -2

Lectures: 60
Max. Marks: 80

COURSE OBJECRTIVES: The main objective of the course is to impart basic knowledge of various laws of thermodynamics, thermodynamics of colligative properties, partial molar properties, affinity, fugacity and activity. This course will also impart knowledge and understanding of solution thermodynamic concepts to compute phase diagram, distribution law, non equilibrium thermodynamics and colloidal state of the system.

Note: *Ten questions will be set by the examiner selecting* ***TWO*** *from each unit. As far as possible every question will be divided into* ***Two – Three Parts****. The students shall attempt* ***FIVE*** *questions selecting* ***ONE*** *from each unit.*

UNIT – I
Chemical Thermodynamics-I: Brief resume of laws of thermodynamics, Free energy functions, Gibb's and Helmholtz free energy functions and their significance, Gibbs -Helmholtz equation, thermodynamic equilibria and free energy functions, applications of Gibbs-Helmholtz equation, Clapeyron-Clausius equation, Thermodynamics of Elevation in boiling point, depression in freezing point, relation between osmotic pressure and elevation of boiling point, relation between osmotic pressure and depression in freezing point.

UNIT – II
Chemical Thermodynamics-II: Chemical affinity, applications of chemical affinity, methods for determining the chemical affinity ,partial molar properties, Physical significance of partial molar properties, chemical potential, Gibbs - Duhem equation, variation of chemical potential with temperature and pressure, chemical potential of a pure solid or liquid, chemical potential of a pure ideal gas and mixture of ideal gases, thermodynamic functions of mixing, fugacity, fugacity coefficient, determination of fugacity, variation of fugacity with temperature and pressure, Lewis Randall rule, Duhem-Margules equation, activity, activity coefficient, determination of activity and variation with temperature and pressure.

UNIT–III
Nernst heat theorem and third law of thermodynamics and its application. Thermodynamic derivation of phase rule and its application to two component systems. Distribution law, its thermodynamic derivation and application.

UNIT –IV
Non–Equilibrium Thermodynamics: Basic principles of non – equilibrium thermodynamics: Rate laws, second law of thermodynamics for open system, law of conservation of mass, charge and energy flow, electrokinetic phenomena and expressions for streaming potential, electro- osmotic pressure difference, streaming potential using the linear phenomenological equation.

UNIT – V
Colloidal State: Classification of colloids, charge and stability of colloidal dispersions, Hardy-Schulze Law, gold number, electrical properties of colloids, electrical double layer and its structure, Stern's theory of double layer, zeta-potential, electrophoresis and electro-osmosis, emulsions and their classification, emulsifiers, gels and their classification.

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
9. Physical chemistry: P.W. Attkin.
10. Introduction to colloid and surface chemistry / Duncan J. Shaw

Course Outcomes:
CO1: Explain principles of laws of thermodynamics and other phenomenon of Chemical Thermodynamics.
CO2: Use of laws of Chemical Thermodynamics to derive other thermodynamic properties.
CO3: Solve problems by choosing suitable thermodynamic derivations and relations.
CO4: Understand the basic laws of non-equilibrium thermodynamics and various electro-kinetic phenomenon.
CO5: Know about the colloidal state of the matter and various electrical properties of colloids.

SEMESTER-II
CHEM 204
Chemistry of life science

Lectures: 48
Max. Marks: 40

COURSE OBJECRTIVES: The main objectives of the course is to learn the basic concepts of biological systems and to understand the fundamentals of cell structure, functions and different metabolic processes involved in cells. It will also impart the knowledge about the role of carbohydrates, proteins, lipids and nucleic acids in biological system.

Note: *Ten questions will be set by the examiner selecting* ***TWO*** *from each unit. As far as possible, every question will be divided into* ***Two – Three Parts****. The students shall attempt* ***FIVE*** *questions selecting* ***ONE*** *from each unit.*

UNIT-I
Cell structure and function: Basic concepts, Structure of prokaryotic and eukaryotic cells, intracellular organelles and their functions, comparison of plant and animal cells.

UNIT-II
Carbohydrates: Structure and biological functions of important monosaccharides (excluding detailed conformational analysis), Disaccharides- sucrose, lactose and maltose, and polysaccharides (cellulose and chitin).

UNIT-III
Carbohydrate Metabolism: Overview of metabolic processes (catabolic and anabolic), energy transfer processes, role and significance of ATP (the biological energy currency). Carbohydrate metabolism: glycolysis and Kreb's cycle.

UNIT-IV
Proteins and lipids: Amino acids, Peptide bond, Chemical and enzymatic hydrolysis of proteins to peptides, Denaturation of Proteins. Biosynthesis of proteins.
Lipid aggregates-micelles, bilayers, and their possible biological functions. Biological membranes. . Introductory idea of metabolism of proteins and lipids

UNIT-V
Nucleic acids: Purine and pyrimidine bases of nucleic acids, base pairing via H-bonding. Structure of ribonucleic acids (RNA) and deoxyribonucleic acids (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 Recommended:

1. Principles of Biochemistry, A. L. Lehninger, Worth Publishers.
2. Biochemistry, L.Stryer, W.H. Freeman.
3. Biochemistry, J. David Rawn, Neil Patterson.
4. Biochemistry, Voet and Voet, John Wiley.
5. Outlines of Biochemistry, E. E.Conn and P. K. Stumpf, John Wiley.
6. Introduction to Chemistry of Life-H.J.DeBay

Course outcome :
CO1: Understand the cell structure, functions and different metabolic processes involved in cells.
CO2: Explain the structure and biological functions of carbohydrates and proteins.
CO3: Know the role of various biological membranes.
CO4: Understand the structure of DNA and RNA and their role in cell replication.
CO5: Explain the structure and bonding of nucleic acids and can explain different enzymatic and chemical processes involved.

SEMESTER-II
CHEM–205
Environmental Chemistry

Lectures: 48
Max. Marks: 40

Course objectives: The main objective of this course is **t**o know the various environmental segments and their chemical composition and to impart the basic knowledge about the air, water, and soil pollution. To create awareness among the students about their ill effects. To understand the basis techniques to monitor environmental pollution along with basic knowledge of green approach in chemical synthesis.

Note: *Ten questions will be set by the examiner selecting* ***TWO*** *from each unit. As far as possible, every question will be divided into* ***Two – Three Parts****. The students shall attempt* ***FIVE*** *questions selecting* ***ONE*** *from each unit.*

UNIT-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.

UNIT-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.

UNIT-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), Biochemical effects of As, Cd, Hg, Pb, Cr, CN and pesticides.
Lithosphere: Soil composition, micro and macro nutrients, soil pollution-fertilizers, pesticides.

UNIT-IV
Environmental analytic chemistry: Introduction to analytical methods for monitoring air and water pollution. Theory and applications of Atomic absorption spectroscopy, UV-Visible and Infrared Spectroscopy, HPLC (High performance liquid chromatography) and Gas chromatography techniques used in pollution analysis.

UNIT-V
Green Chemistry: Introduction and need for Green Chemistry. Goals of Green Chemistry. Principles of Green Chemistry with their explanations. Green chemistry in sustainable development.

Books recommended
[1] Environmental Chemistry-A.K.De
[2] Environmental Chemistry-Manaham
[3] Environmental Pollution Analysis-Khopkar
[4] Vogel's text book of Quantitative Chemical Analyses.
[5] Ahluwalia, V.K. and Kidwai, M.R. New Trends in Green Chemistry, Anamalaya Publishers, 2005
[6] Matlack, A.S. Introduction to Green Chemistry, Marcel Dekker, 2001

Course outcomes:
CO1: Analyze composition of atmosphere, hydrosphere and lithosphere and pollution involved and waste water treatment methods.
CO2:Understand the fundamentals of environmental analysis.
CO3: Identify different types of analytical methods and to apply them to analyze air and water pollution.
CO4: Analyse composition of atmosphere, hydrosphere, lithosphere and pollution involved and waste water treatment methods.
CO5: To understand the need of green chemistry and its principles

SEMESTER II
CHEM 206
Inorganic Chemistry Practical -2

Time - 6 hr/week
Max. Marks -50

Course Objectives: The Course is introduced to impart students with practical knowledge of the chemical methods of analysis along with green methods of synthesis with a view to develop their experimental skills and creativity.

1. 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)
8. Analysis of Ores (Dolomite, Pyrolusite) and alloys (Coin, Brass, Bronze).

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.

2. **Green methods of Preparation of the following:**

(i) Bis(acetylacetonato)copper(II)
(ii) Tris(acetylacetonato)iron(III)
(iii) Tris(acetylacetonato)manganese(III)

Books Recommended:

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

Course Outcomes:

CO 1: Demonstrate the application of chemical method in commercial analysis of industrial products as quality control measure.
CO 2: To understand the various measures to control environmental pollution by some green synthesis experiments as alternative to conventional methods.
CO 3: To perform experimentation and evaluate the results.
CO 4: Develop the ability to compile interpreted information in the form of lab record and to face viva-voce

SEMESTER II
CHEM- 207
Organic Chemistry Practical -2

Time : 6 hr/week
Max. Marks : 50

Course Objectives: The main objective of this course is to provide basic knowledge of principle and techniques of separation, purification and identification of binary mixture of organic compounds. To understand and develop the capabilities of preparing derivatives of different organic compounds bearing various organic functionalities. To know the significance of melting point mixed melting point, boiling point in identification of organic compounds

Qualitative Organic Mixture Analysis: Separation, purification and identification of binary mixture of organic compounds by chemical tests. Separation of binary mixtures: using H_2O, HCl, NaOH, $NaHCO_3$, Ether or other reagent as may be necessary along with required conditions for their use.
Systematic identification of mixtures of pure organic compounds: separation and identification of simple binary mixtures having acidic, basic and neutral components. Preparation of their derivatives, determination of b.p./m.p. for components and their derivatives.
Any other experiment to be added as per requirement.

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.

Course Outcomes:
CO1: Describe and demonstrate the basic principle and techniques of separation of binary organic mixture.
CO2: Analyse qualitatively the presence of extra elements and functional groups in the binary organic mixture along with understanding of chemical reaction involved.
CO3: Understand and develop the capabilities of preparing derivatives of different organic
CO4: Understand significance of melting point mixed melting point, boiling point in identification of organic compounds.
CO5: Develop the ability to compile interpreted information in the form of lab record and to face the viva-voce.

SEMESTER II
CHEM 208
Physical Chemistry Practical -2

Time - 6 hr/week
Max. Marks - 50

COURSE OBJECTIVES: This course will impart basic knowledge of various methods used for the determination of partition coefficient, heat of neutralisation, heat of solution and heat of hydration. This course will also impart knowledge and understanding for the verification of Freundlich adsorption isotherm, preparation of sol and construction of Phase diagrams for liquids

1. **Partition – Coefficient**: Determination of partition – coefficient for iodine (I_2) and benzoic acid between two immiscible solvents.

2. **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.

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

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

5. **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).

Books Recommended:

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

COURSE OUTCOMES:

CO1: Understand the safe handling of chemicals and safety measures to be followed in the labs.
CO2: Use various methods in determining partition coefficient of iodine between two immiscible liquids
CO3: Determine heat of neutralisation and heat of solution for different acid and base combinations
CO4: Verify the Freundlich Adsorption Isotherm for I_2, and acetic acid on charcoal
CO5: Prepare the colloidal solution arsenic sulphide
CO6: Construct phase diagrams for liquids and solids

SEMESTER-III
CHEM 301
Inorganic Chemistry Theory -3

Lectures-60
Max. Marks-80

Course Objectives: The Course is introduced to provide basic to advance level of knowledge to student like bonding considerations in metal pi complexes, statistical treatment of analytical data, transuranium and translawrencium elements and photoelectron spectroscopy and applications of nuclear chemistry.

Note: *Ten questions will be set by the examiner selecting* ***TWO*** *from each unit. As far as possible, every question will be divided into* ***Two – Three Parts****. The students shall attempt* ***FIVE*** *questions selecting* ***ONE*** *from each unit.*

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

UNIT-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.

UNIT-III
Photoelectron Spectroscopy: Basic principle, photoionization process, ionization energies, Koopman's theorem, ESCA, photoelectron spectra of simple molecules, (N_2, O_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.

UNIT-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.

UNIT-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

Course Outcomes:
CO 1:Explain the various aspects of and properties of metal-pi complexes of transition metals.
CO 2: Describe basic concept of analytical Chemistry and apply the same to data analysis.
CO 3: Understand and explain the basic principle of photoelectron spectroscopy.
CO 4: Explain the spectral and magnetic properties of lanthanide and Actinide compound.
CO 5: Apply the basic concepts of nuclear chemistry to explain, nuclear reactions and radioactive techniques.

SEMESTER-III
CHEM 302
Organic Chemistry Theory -3

Lectures: 60
Max. Marks: 80

Course Objectives: The main aim of the course is to provide the basic knowledge about the principles and instrumentation of spectroscopic techniques like ultra violet-visible spectroscopy, infrared spectroscopy, nuclear magnetic resonance (NMR) spectroscopy and mass spectrometry along with their application for the structure elucidation of organic compounds. This course will also provide the knowledge about the basic principles of photochemistry and photochemical reactions.

Note: *Ten questions will be set by the examiner selecting* ***TWO*** *from each unit. As far as possible every question will be divided into* ***Two – Three Parts****. The students shall attempt* ***FIVE*** *questions selecting* ***ONE*** *from each unit.*

Unit -I
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, Steric effect in biphenyls, Fieser- Woodward rules for conjugated dienes and carbonyl compounds, ultra violet spectra of aromatic and heterocyclic compounds.. Applications of UV- visible spectroscopy in organic chemistry.

Unit -II
Infrared Spectroscopy: Principle, 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.

Unit -III
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. First and second order spectra, 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 –^{13}C NMR, 2-D and 3-D NMR, Applications of NMR in organic chemistry.

Unit -IV
Mass Spectrometry: Introduction, ion production—EI, CI, FD and FAB, factors affecting fragmentation, ion analysis, and ion abundance. Mass spectral fragmentation of organic compounds with common functional groups, Molecular ion peak, Meta-stable peak, McLafferty rearrangement. Nitrogen Rule. 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.

Unit -V
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
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.
16. Spectroscopy by Pavia

Course Outcomes:
CO1: Apply the basic concepts of Ultraviolet and Visible Spectroscopy and its applications.
CO2: Understand the basic principle of IR spectroscopy and its applications.
CO3: Understand the basic principle of NMR spectroscopy and to apply its role for the structure elucidation.
CO4:Apply the concept of mass spectrometry for the determination of structure of organic compounds based on fragmentation.
CO5: Understand the basic principles of photochemistry and various photochemical reactions.

SEMESTER-III
CHEM 303
Physical Chemistry Theory -3

Lectures: 60
Max. Marks: 80

COURSE OBJECRTIVES: This course is introduced to impart students with the knowledge of terms and concepts used in statistical thermodynamics, partition functions and theories. This course also imparts knowledge and understanding of basics of quantum chemistry and other photophysical processes.

Note: *Ten questions will be set by the examiner selecting **TWO** from each unit. As far as possible every question will be divided into **Two – Three Parts**. The students shall attempt **FIVE** questions selecting **ONE** from each unit.*

Statistical Thermodynamics
UNIT – I
Basic Terminology: probability, phase space, micro and macro states, thermodynamic probability, statistical weight, assembly, ensemble, 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 and its importance.
Applications to ideal gases: The molecular partition function and its factorization. Evaluation of translational, rotational and vibrational partition functions, the electronic and nuclear partition functions. for monatomic, diatomic and polyatomic gases.

UNIT – II
Thermodynamic properties of molecules from partition function: Total energy, entropy, Helmholtz free energy, pressure, heat content, heat capacity and Gibb's free energy, equilibrium constant and partition function, Heat capacity of crystals and statistical thermodynamics, Third law of thermodynamics and entropy. Ortho- and para-hydrogen, statistical weights of ortho and para states, symmetry number. Calculation of equilibrium constants of gaseous solutions in terms of partition function, Einstein theory and Debye theory of heat capacities of monatomic solids.

Basic Quantum Chemistry

UNIT – III
Operators in quantum mechanics. Introduction to angular momentum. Eignvalues and eignfunctions. Hermitian operator. Postulates of quantum mechanics. Time dependent and time independent Schrodinger wave equations.

UNIT – IV
Some analytically soluble problems (complete solutions) of particle in a one and three dimensional box, harmonic – oscillator, the rigid rotor, the hydrogen atom and the quantum mechanical tunnelling.

Photochemistry

UNIT – V
Photophysical processes of electronically excited molecules (Jablonski Diagram). Franck-Condon principle. Kinetics of Excimer and exciplex formation. Energy transfer from electronically excited molecules (Stern – Volmer mechanism). E- type and P- type delayed fluorescence.

Suggested Reading:
1. Physical Chemistry: P.W. Atkins
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

By the end of the course, students will be able to
CO1: explain various terms and concepts used in statistical thermodynamics
CO2:use of concepts of statistical thermodynamics to derive various expressions and equations
CO3: solve problems by using suitable statistical thermodynamic relations and equations
CO4: understand the basics of quantum chemistry and their use in solving various problems
CO5: know about the various photophysical processes and their kinetics

SEMESTER-III
CHEM 304
Inorganic Chemistry Special Theory -1

Lectures-60
Max. Marks-80

Course Objectives: The objective of this course is to provide advance level of specialized knowledge in inorganic chemistry to student regarding photochemistry, reaction mechanism and polymeric inorganic compounds and electronic spectra of complex ions. The concept of stability of inorganic compounds and their determination by various techniques has also been incorporated which will be helpful in synthesizing new compounds.

Note: *Ten questions will be set by the examiner selecting* ***TWO*** *from each unit. As far as possible, every question will be subdivided into* ***Two – Three Parts****. The students shall attempt* ***FIVE*** *questions selecting* ***ONE*** *from each unit.*

UNIT-I
Inorganic Photochemistry: Basic principles, absorption, excitation, kasha rule, electronically excited state, its life-time and energy dissipation process. Photochemical behavior of transition metal complexes, charge transfer spectraof crystalline and gasous alkali halides. Photochemistry of chromium(III) octahedral complexes, $[Cr(H_2O)_6]^{3+}$ and $[Cr(NH_3)_6]^{3+}$. Photochemistry of cobalt (III) complexes, $[Co(NH_3)_5X]^{2+}$ and $[Co(en)_3]^{3+}$.

UNIT-II
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.

UNIT-III
Polymeric Inorganic Compounds: General chemical aspects (synthesis, properties and structure)of phosphazenes, borazines, silicones, sulphur- nitrogen cyclic compounds and condensedphosphates.

UNIT-IV
Stability of Coordination Compounds – Stability constants, stepwise formation constants, overall formation constants, relationship between stepwise and overall formation constants, factors affecting the stability constants (with special reference to metal and ligand ions), Difference between thermodynamic and kinetic stability. Determination of stability constants by:
(i) Spectrophotometric methods (Job's method, Mole ratio and slope ratiomethod).
(ii) Bjerrum's method
(iii) Polarographic method

UNIT-V
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 d1-d9 ions in Oh and Td environments, Evaluation of 10 Dq, Spectrochemical and Nephelauxetic series, charge- transfer spectra.

Books Recommended:

1. Instability Constants- Yttermiskii
2. Advanced Inorganic Chemistry- Cotton and Wilkinson
3. Inorganic Chemistry- T.Moeller
4. Concise Inorganic Chemistry- J.D.Lee
5. Introduction to Ligand Fields- B.N.Figgis
6. Modern Aspects of Inorganic Chemistry-H.J.Emeleus and A.G.Sharpe
7. Inorganic chemistry: A Unified Approach W.W.Porterfield
8. Inorganic Reaction Mechanism – Edberg
9. Inorganic Reaction Mechanism – BasoloavdPearsor

Course Outcomes:
CO 1: Apply the basic principles of inorganic photochemistry to explain the transition metal complexes.
CO 2: Explain the inorganic reactions and mechanism of transition metal complexes.
CO 3: Explain general aspects and classification of inorganic polymers and their comparison with organic polymers with application.
CO 4: Understand and explain the kinetic and thermodynamic stability coordination compounds.
CO 5: Analyze electronic spectra of transition metal complex ions.

SEMESTER-III
CHEM 305
Organic Chemistry Special Theory -1

Lectures: 60
Max. Marks: 80

Course Objectives: The main objective of this course is to provide basic knowledge of biochemistry to the students regarding some biomolecules including carbohydrate, proteins, vitamins, enzymes and coenzymes. To provide knowledge about the enzyme catalyzed reactions, mechanism of enzyme action and various theories of enzyme catalysis. To get knowledge about coenzymes derived from vitamins and their structure and biological functions. To understand the mechanism of biochemical reaction catalysed by coenzymes.

Note: *Ten questions will be set by the examiner selecting* ***TWO*** *from each unit. As far as possible every question will be divided into* ***Two – Three Parts****. The students shall attempt* ***FIVE*** *questions selecting* ***ONE*** *from each unit.*

Unit-I
Carbohydrates: Types of naturally occurring sugars: Deoxy-sugars, amino sugars, branched chain sugars. General methods of structure and ring size determination with particular reference to maltose, lactose, sucrose, pectin, starch and cellulose, photosynthesis of carbohydrates, metabolism of glucose, Glycoside- (amygdalin).

Unit-II
Amino acid, peptides and proteins: General methods of peptide synthesis, sequence determination. Chemistry of insulin and oxytocin. Purines and nucleic acid. Chemistry of uric acid, adenine, protein synthesis.

Unit-III
Vitamins: A general study, detailed study of chemistry of thiamine (Vitamin B1), Ascorbic acid (Vitamin C), Pantothenic acid, biotin (Vitamin H), α-tocopherol (Vitamin E), Biological importance of vitamins.

Unit-IV
Enzymes: Remarkable properties of enzymes like catalytic power, specificity and regulation, Mechanism of enzyme action: Proximity effects and molecular adaptation, Chemical and biological catalysis, Transition state theory, orientation and steric effects, acid base catalysis, covalent catalysis, strain or distortion. Examples of some typical enzyme mechanisms (chymotrypsin, ribo nuclease, lysozyme and carboxypeptidase A). Fischer's lock and key and Koshland's induced fit hypothesis, Enzyme kinetics, Michaelis-Menten and Lineweaver-Burk plots, reversible and irreversible inhibition.

Unit-V
Coenzyme Chemistry: Cofactors as derived from vitamins, coenzymes, prosthetic groups, and apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD^+, $NADP^+$, FMN, FAD, Lipoic acid, vitamin B_{12}. Mechanism of reactions catalyzed by the above coenzymes.

Books recommended:

1. Bioinorganic Chemistry: A Chemical Approach to Enzyme Action, Herman Duags and C. Penny, and Springer-Verlag.
2. Understanding Enzymes, Trevor Palmer, Prentice Hall.
3. Enzyme Chemistry; Impact and Applications, Ed. Collin J Suckling, Chapman and Hall.
4. Enzyme Mechanisms Ed, M.I. Page and A. Williams, Royal Society Of Chemistry.
5. Fundamentals of Enzymology, N.C. Price and L. Stevens, Oxford Univ. Press.
6. Immobilized Enzymes: An Introduction and Applications In Biotechnology, Michael D. Trevan, John Wiley.
7. Enzymatic Reaction Mechanisms. C. Walsh, W. H, Freeman.
8. Enzyme Structure and Mechanism, A. Fersht, W.H. Freeman.
9. Biochemistry the Chemical Reactions of Living Cells, D.E. Metzler, Academic Press.
10. Carbohydrates by N. Sharon.
11. Carbohydrates by Gutherie.
12. Carbohydrates by Pigman and Wolfrom.
13. The Nucleic Acids (Vol I-III) by Chargoff and Davidson.
14. Protein Structures and Functions by A. Light.
15. Chemistry of Natural Products Vol. I by K. Nakanishi.
16. Peptides and Amino Acids by R.H. Thomson.
17. The chemistry of Natural Products by P.S. Kalsi.

Course Outcomes:
CO1: Know about carbohydrates and methods of structure and ring size determination.
CO2: Understanding about general methods of peptide synthesis, sequence determination and protein synthesis.
CO3: Explain the structure of enzymes, properties of enzymes, mechanism and theories of enzyme action.
CO4: Understand the structure, biological function and method of structure determinations of vitamins.
CO5: Understand the mechanistic implications of the reactions catalysed by the coenzymes.

SEMESTER-III
CHEM 306
Physical Chemistry Special Theory -1

Lectures: 60
Max. Marks: 80

COURSE OBJECRTIVES: This course is introduced to impart students with the knowledge of various mechanisms of adsorption at solid – gas interface and solid – liquid interface. This course also imparts knowledge and understanding of solutions and interfacial behaviour of surfactants, theories and laws of electrochemistry and chemistry of nanomaterials.

Note: *Ten questions will be set by the examiner selecting* ***TWO*** *from each unit. As far as possible, every question will be divided into* ***Two – Three Parts****. The students shall attempt* ***FIVE*** *questions selecting* ***ONE*** *from each unit.*

UNIT –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.

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

UNIT –III
Solution and Interfacial Behaviour of Surfactants: Definition and classification of surfactants. Solution properties of surfactants: micelle formation, critical micelle concentration (CMC), dependence of CMC on chain length of the surfactant, micelle shape and size. 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.

UNIT –IV
Electrochemistry: Quantitative treatment of Debye - Hückel and Debye-Hückel-Onsagar (D-H-O) theory of conductance of electrolyte solution their limitations and modifications. Pair-wise association of ions (Bjerrum and Fuoss treatment). Determination of association constant (KA) from Debye – Huckel Limiting Law. Extended Debye – Huckel Law. Qualitative treatment of ion – solvent interactions (ion solvation).

UNIT –V
Chemistry of nano – materials: Definition and historical perspective. Effect of nanoscience and nanotechnology in various fields. Synthesis of nanoparticles by chemical routs and their characterization techniques. Properties of nanostructured material: optical, magnetic and chemical properties. An overview of applied chemistry of nanometerials.

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

Course Outcomes:
CO1: explain various adsorption processes at solid – gas interface and solid-liquid interfaces
CO2: use of various phenomenon to derive various expressions and equations involving adsorption
CO3: solve problems by using suitable expressions and equations involving adsorption
CO4: understand the solution properties and interfacial behaviour of surfactants and their practical applications
CO5: know about the various theories and laws of electrochemistry
CO6: apply applications of nano chemistry in fabricating some useful nanomaterials.

SEMESTER III
CHEM 307
Inorganic Chemistry Practical -3

Time - 6 hr/week
Max. Marks –50

Course Objectives: This practical Course is introduced to impart students with practical knowledge of the various methods of synthesis of inorganic compounds and their subsequent characterization by elemental analysis, molar conductance and thermal analysis and spectral techniques.This training is very important for any synthetic chemists involved in the synthesis of new compounds for varied applications and thus will help to develop their experimental skills and creativity.

Preparation of following compounds:
1. Tetrapyridine copper (II) persulphate
2. Dinitritotetrapyridine nickel (II)
3. Mercury (tetraisothiocyanato)cobaltate(II).
4. Potassium tris(oxalato)aluminate(III)
5. Sodium hexa(nitro)cobaltate(III)
6. Potassium tris(oxalato)cobaltate(III)
7. Hexa(ammine)cobalt (III)chloride

Characterization of above compounds 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
2. Synthetic Coordination Chemistry: Principles and Practice- J.A. Davies, C.M. Hockensmith, V.Y.Kukushkin and Y.N. Kukushkin.

Course Outcomes:
CO1: Know about carbohydrates and methods of structure and ring size determination.
CO2: Understanding about general methods of peptide synthesis, sequence determination and protein synthesis.
CO3:Explain the structure of enzymes, properties of enzymes, mechanism and theories of enzyme action.
CO4: Understand the structure, biological function and method of structure determinations of vitamins.
CO5: Understand the mechanistic implications of the reactions catalysed by the coenzymes.

SEMESTER III
CHEM 308
Organic Chemistry Practical -3

Time : 6 hr/week
Max. Marks : 50

Course Objectives: The main objectives of the practical course are to understand the basics of quantitative analysis and application in analysis of functional groups in organic compounds. To understand the concept of stepwise synthesis of a product and their purification. To know the practical applicability of different types of organic reactions.

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.
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→ Benzophenone oxime →Benzanilide.
Skraup Synthesis: Preparation of quinoline from aniline.
Synthesis using Phase Transfer Catalysis: Alkylation of diethyl malonate or ethyl acetoacetate and an alkyl halide.
Synthesis of p- nitro aniline and any other reaction as per requirement.
TLC and column chromatography.
All the students must submit the recrystallised product along with yield, melting point and R_f value for all the stages of preparation

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.

Course Outcomes:
CO 1: Apply the basic concepts of quantitative analysis to analyze the functional groups in organic compounds.
CO 2: Understand the concept of stepwise synthesis of a product and their purification.
CO 3: Perform experimentation and evaluate the results.
CO 4: Develop the ability to compile interpreted information in the form of lab record.
CO 5: Know about how to face viva-voce.

SEMESTER III
CHEM 309
Physical Chemistry Practical -3

Time - 6 hr/week
Max. Marks - 50

COURSE OBJECTIVES: This course is introduced to impart knowledge of various experimental methods and techniques used for the determination of heat of solution and heat of transfer for various electrolytes. This course will also impart knowledge and understanding of various conductometric measurements and including verification of verification of Beer – Lambert's law for various aqueous solutions.

1. **Solubility Measurements:**Heat of solution of electrolytes by solubility measurements.
2. **Heat of transfer Measurements:** Heat of transfer for benzoic acid and I_2 between two immiscible solvents.
3. **Conductometric Measurements:** Determination of cell constant, limiting molar conductance of simple electrolytes in water, verification of Ostwald, dilution law for week acetic acid.
4. **Conductometric Titrations:** Precipitation, and acid base titration., determination of relative strength of acids in the given mixtures of acids, solubility of sparingly soluble salt.
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.

Books Recommended:

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

Course Outcomes:

CO1: understand the safe handling of chemicals and safety measures to be followed during the laboratory
CO2: determine heat of solution and heat of transfer for various electrolytes
CO3: determine cell constant and limiting molar conductance of simple electrolytes in water
CO4: compare the relative strength of acids in the given mixtures conductometrically
CO5: determine the solubility of sparingly soluble salt by conductometric titrations.
CO5: verify Beer-Lambert's law for different aqueous solutions

SEMESTER-IV
CHEM 401
Inorganic Chemistry Special Theory -2
(Advanced Organometallics)

Lectures-60
Max. Marks-80

Course Objectives: The objectives of this course is to provide advance knowledge in one of the fast growing fields in inorganic chemistry. The course covers all the aspects of the chemistry of organometallics starting from synthesis and structural considerations to their applications as homogeneous catalysts including mechanism and other applications in biological field. The structural chemistry of carbonyl clusters and metal multiply bonded to carbon are also included.

Note: *Ten questions will be set by the examiner selecting **TWO** from each unit. As far as possible every question will be divided into **Two – Three Parts**. The students shall attempt **FIVE** questions selecting **ONE** from each unit.*

UNIT-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 Organometallic compounds (classification)

UNIT-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 igration and elimination, rearrangement). Phase transfer catalysis. Homogeneous hydrogenation of unsaturated compounds (alkenes, alkynes, aldehydes and ketones). Asymmetric hydrogenation (Olefins).

UNIT-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, carbonylation of alkenes and alkynes using nickel carbonyl and palladium complexes.

UNIT-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.

UNIT-V
Transition Metal-Carbon multiple bonded compounds:-Metal carbenes and carbines (preparation, reactions, structure and bonding considerations). Biological and industrial applications, and environmental aspects of organometallic compounds.

Books Recommended:

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

Course Outcomes:
CO1:Classify organometallic compounds and describe the bonding and fluxionality in organometallic compounds of transition elements.
CO2:Understand various aspects of homogeneous transition metal catalysis and apply them to explain hydrogenation of organic compounds. .
CO3:Explain important homogeneous catalytic reactions and their utility in organic synthesis.
CO4:Classify metal clusters and explain metal-metal bonding in metal clusters.
CO5:Apply different aspects the metal-carbon multiple bonded organometallic compounds and their different applications.

SEMESTER-IV
CHEM 402
Inorganic Chemistry Special Theory -3
(Modern Techniques of Chemical Analysis)

Lectures-60
Max. Marks-80

Course Objectives: The key objective to frame this course is to acquire a foundational understanding of various analytical techniques employed in quantitation of chemical compounds. As part of this course, students will be introduced to optical, electro analytical, chromatographic and thermal techniques of analysis with detailed description of instrumentation, principle and applications in various fields.

Note: *Ten questions will be set by the examiner selecting* ***TWO*** *from each unit. As far as possible, every question will be subdivided into* ***Two – Three Parts****. The students shall attempt* ***FIVE*** *questions selecting* ***ONE*** *from each unit.*

UNIT-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.

UNIT-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.

UNIT-III
Chromatographic methods: Introduction, terminology and basic principleclassification of chromatographic methods. Chromatographic behavior of solutes. Column efficiency and resolution. Instrumentation, columns, solvent systems and detection methods and applications and comparison ofGas chromatography (GC) and High-Performance Liquid Chromatography (HPLC).

UNIT-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.

UNIT-V
Thermoanalytical methods: (a) Thermogravimatric analysis: Introduction, Factors affecting thermogravimetric curves, Instrumentation, Applications to inorganic compounds (analysis of Ca and Mg in binary mixture, calcium oxalate, determination of Ca, Sr & Ba in the mixture, drying of sodium carbonate) and analysis of clays and soils, and determination of titanium content of non-stoichiometric sample of titanium carbide).
(b) ***Differential thermal analysis:*** Introduction, Factors affecting DTA curves, Instrumentation, Applications to inorganic compounds : Mixtures of lanthanum-cerium and praseodymium oxalate, CuSO4.5H2O, detection of organic contamination in ammonium nitrate, different magnesium carbonate samples and 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. Fundamentals of Analytical Chemistry – Skoog , West, Holler and Crouch.
3. Instrumental Methods of Chemcial Analysis-G.K.Ewring
4. Modern Polarographic Methods in Analytical Chemistry -A.M.Bond
5. Thermal Methods of Analysis-W.W. Wendlandt.

Course Outcomes:
CO 1:Understand the fundamental laws of absorption, photometric titrations, molecular fluorescence spectroscopy and their applications in quantitative analysis.
CO 2:Describe the different types absorption and emission spectroscopy and removal of interferences.
CO 3: Understand and explain the separation techniques with reference to chromatography and their applications.
CO 4: Explain general aspects of polarography and its applications to inorganic and organic quantitative analysis.
CO 5:Describe thermoanalytical techniques and their applications to the analysis of Inorganic compounds.

SEMESTER-IV
CHEM 403
Inorganic Chemistry Special Theory -4
(Inorganic Spectroscopy)

Lectures-60
Max. Marks-80

Course Objectives: Spectroscopy is one of the versatile field in chemistry and other science streams.This course is designed to provide application of spectroscopy in inorganic chemistry for characterization purposes very valuable tool in synthetic inorganic chemistry. The most commonly used techniques like IR, NMR,ESR,Mossbaur and NQR have thus been included with a view the students can use them in their research and scientific jobs.

Note: *Ten questions will be set by the examiner selecting **TWO** from each unit. As far as possible, every question will be divided into **Two – Three Parts**. The students shall attempt **FIVE** questions selecting **ONE** from each unit.*

UNIT-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.
Applications 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) Modes of bonding of ligands such as urea and dimethylsulphoxide.

UNIT-II
Nuclear Magnetic Resonance Spectroscopy: Introduction, Chemical shift, Mechanism of electron shielding and factors contributing to the magnitude of chemical shift, Nuclear overhausser effect, Double resonance, Chemical exchange, Lanthanide shift reagents and NMR spectra of paramagnetic complexes. Experimental techniques (CW and FT).
Stereochemical non-rigidity and fluxionality: Introduction, use of NMR in its detection in PF_5, $Ti(acac)_2Cl_2$, $Ti(acac)_2Br_2$, $Ta_2(OMe)_{10}$.

UNIT-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. Structural information of the following: PCl5, TeCl4, Na^+GaCl4^-, BrCN, and Hexahalometallates

UNIT-IV
Mössbauer Spectroscopy: Introduction**,** Principle, Conditions for Mössbauer Spectroscopy, Parameters from Mössbauer Spectra- Isomer shift, Electric Quadrupole Interactions, Magnetic Interactions, MB instrumentation, Applications of MB spectroscopy in structural determination of the following:

i) High spin Fe (II) and Fe (III) halides- FeF2, FeCl2.2H2O, FeF3, FeCl3.6H2O.
ii) Low spin Fe(II) and Fe(III) Complexes- Ferrocyanides, Ferricyanides, Prussian Blue.
iii) Iron carbonyls. Fe(CO)5, Fe2(CO)9 and Fe3 (CO)12
iv) Inorganic Sn(II) and Sn(IV) halides.

UNIT-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

Course Outcome
CO 1: Explain the principle IR spectroscopy and its use in characterization of inorganic compounds
CO 2:Explain the basic aspects of NMR spectroscopy and its application for detection of inorganic compounds.
CO 3: Discuss basic concepts of NQR spectroscopy and its application in inorganic chemistry.
CO 4: Apply basic concepts of Mossbauer spectroscopy and its application in inorganic chemistry.
CO 5: Explain the basic principle of ESR spectroscopy and its significance in transition metal complexes.

SEMESTER-IV
CHEM 404
Inorganic Chemistry Special Theory -5
(Bio-Inorganic Chemistry)

Lectures-60
Max. Marks-80

Course Objectives: The goal of this course is to teach the fundamentals of bio inorganic chemistry at master level. A variety of topics will be covered that are important in biological system and is the fast growing interdisciplinary science. The course aims to impart knowledge of the concepts related to transport and storage of metals, oxygen carriers, enzymes, nitrogen fixation. The current trends of the use of inorganic compounds as biologically active compounds.are gaining importance and hence this course will help students to peruse their research programme.

***Note:** Ten questions will be set by the examiner selecting **TWO** from each unit. As far as possible, every question will be divided into **Two – Three Parts**. The students shall attempt **FIVE** questions selecting **ONE** from each unit.*

UNIT-I
(a) 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).
(b) Metalloenzymes: Definitions: Apoenzyme, Coenzyme, Metalloenzyme, structure and functions of Carboxy peptidases and Carbonic anhydrase.

UNIT-II
Oxygen Carriers: a) *Natural oxygen carriers:* Structure of hemoglobin and myoglobin, Bohr effect, Models for cooperative interaction in hemoglobin, oxygen Transport in human body (-perutzmachanism), Cyanide poisoning and its remedy. Non-heme protiens (Hemerythrin & Hemocyanin).
b) *Synthetic oxygen carriers:* Oxygen molecule and its reduction products, model compounds for oxygen carrier (Vaska's Iridium cjomplex, cobalt complexes with dimethyl glyoxime and Schiff base ligands).

UNIT-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).

UNIT-IV
Inorganic compounds as therapeutic Agents :- Introduction chelation therapy, synthetic metal chelates as antimicrobial agents, antiarthritis drugs, antitumor, anticancer drugs (Platinum complexes), Lithium and mental health.

UNIT-V
Nitrogen fixation :A. Nitrogen molecule (MO picture) and its transition metal complexes, reactivity of coordinated dinitrogen, *in-vivo* and *in-vitro* nitrogen fixation, symbiotic and asymbiotic nitrogen fixation.
B. Nitrogen metabolism : Introduction, elementary idea about nitrogen nutrition in various forms (nitrate and ammonia nitrogen).

Books Recommended:

1. The Inorganic Chemistry of Biological processes - M.N.Hughes.
2. Bio Inorganic Chemistry - Robert Hay
3. Advanced Inorganic Chemistry (4th Edn) - Cotton and Wilkinson.
4. Topics in current chemistry (Inorganic Biochemistry) vol. 64 (1976) – Davison and Coworkers.
5. General Biochemistry - Fruton J.S. and Simmonds S.
6. Plant Physiology - Robert N.Devlin.
7. Inorganic chemistry – James E. Huheey.

Course outcomes:
CO 1:Discuss basic concepts of bioinorganic chemistry and the role of metalloporphyrin, metalloenzymes in biological systems.
CO 2:Discuss natural and synthetic oxygen carriers.
CO 3:Explain the electron transfer processes in living organisms with reference to transport and storage of iron.
CO 4: Explain the therapeutic importance of and chelation therapy of synthetic metal chelates.
CO 5:Explain the importance of nitrogen containing compounds in nutrition and plants.

SEMESTER-IV
CHEM 405
Organic Chemistry Special Theory -2
(Organic Synthesis)

Lectures: 60
Max. Marks: 80

Course Objectives: The basic objective of this course is to understand mechanistic details of different types of oxidation, reduction and rearrangement reactions. As part of this course, students will know about some common reagents used in organic synthesis and their applications. To get knowledge about various terms used in disconnection approach and to apply the concepts of disconnection approach for the synthesis of different target molecules in organic chemistry.

Note: *Ten questions will be set by the examiner selecting* ***TWO*** *from each unit. As far as possible every question will be divided into* ***Two – Three Parts****. The students shall attempt* ***FIVE*** *questions selecting* ***ONE*** *from each unit.*

Unit- 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. Grubbs Catalysts.

Unit- 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

Unit- 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 .

Unit- 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, Baeyer-Villiger, Shapiro reaction, Witting rearrangement and Stevens rearrangement.

Unit- 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. 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, Verlage VCH.
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.

Course Outcomes:
CO1: Explain the mechanistic implications of some common reagents used in organic synthesis and their applications.
CO2: Understand the concept of oxidation reactions and their applications.
CO3: Understand the concept of reduction reactions and their applications.
CO4: Mechanistic implications of rearrangement reactions and their applications
CO5: Apply the concepts of disconnection approach for the synthesis of organic molecules.

SEMESTER-IV
CHEM 406
Organic Chemistry Special Theory -3
(Natural Products)

Lectures: 60
Max. Marks: 80

Course Objectives: To understand general aspects of isolation and structure elucidation of natural products including terpenoids, carotenoids and xanthophylls, alkaloids, steroids and plant Pigments. To provide the knowledge about the synthesis and biosynthesis of these natural products.

Note: *Ten questions will be set by the examiner selecting* ***TWO*** *from each unit. As far as possible every question will be divided into* ***Two – Three Parts****. The students shall attempt* ***FIVE*** *questions selecting* ***ONE*** *from each unit.*

Unit- 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.

Unit- II
Carotenoids and Xanthophylls: General methods of structure determination of Carotenes: β-carotene, α- carotene, γ-carotene, lycopene and vitamin A. Xanthophylls: Capsorubin, Fucoxanthin. Carotenoid acids (Apocarotenoids): Bixin and Crocetin. Bio synthesis of carotenoids

Unit- 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.

Unit- 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

Unit- 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.

Course Outcomes:
CO1: Understand the concept of natural product isolation and structural illucidation terpenoids.
CO2: Apply the general methods of structure elucidation to analyze alkaloids.
CO3: Analyse the structure elucidation methods and biosynthesis of steroids.
CO4: Describe the general methods of structure determination of carotenoids
CO5: Understanding about the general methods of structure determination of some plant pigments.

SEMESTER-IV
CHEM 407
Organic Chemistry Special Theory -4
(Medicinal Chemistry)

Lectures: 60
Max. Marks: 80

Course Objectives: The main objectives of the course is to provide basic as well as advance knowledge of medicinal chemistry. To know about the procedure followed in drug design. To understand the basic concept of lead compound, lead modification, prodrugs and structure-activity relationships. To understand the concepts of drug receptors and various theories of drug activity. To familiarize with pharmacokinetics (ADME) and important pharmacokinetic parameters. To understand pharmacodynamics and significance of drug metabolism in medicinal chemistry. To provide the knowledge about structure-activity relationships (SAR) and mode of action of some antibiotics and anti-infective drugs. To know about the SAR and mode of action of some central nervous system depressant and stimulants drugs, along with some antineoplastic, cardiovascular, antihistaminic, antifertility and diuretics agents.

Note: *Ten questions will be set by the examiner selecting* ***TWO*** *from each unit. As far as possible every question will be divided into* ***Two – Three Parts****. The students shall attempt* ***FIVE*** *questions selecting* ***ONE*** *from each unit.*

Unit- 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 relationships (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. 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. Naming of drugs-Trade names and Generic names

Unit- II
Pharmacokinetics and Pharmacodynamics: Pharmacokinetics: Introduction to drug absorption, distribution, metabolism, elimination using pharmacokinetics. Importance of pharmacokinetic parameters in defining drug distribution and in therapeutics. Importance of pharmacokinetics in drug development process.
Pharmacodynamics : Introduction, elementary treatment of enzyme stimulation, enzyme inhibition, membrane active drugs, drug metabolism, xenobiotics, biotransformation, Significance of drug metabolism in medicinal chemistry.

Unit- III
Antibiotics and Antiinfective Drugs: Antibiotics: Historic development in the structural modifications of Penicillin 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, Sulfaguanidine, Dapsone, Introduction and general mode of action of Local antiinfective drugs, Examples: sulphonamides, furazolidone, ciprofloxacin, norfloxacin, chloroquin and primaquin

Unit- IV
Psychoactive Drugs: Introduction, neurotransmitters-receptor interaction, CNS depressants and stimulants. SAR and Mode of action, 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.

Unit- V
Therapeutic Agents, SAR and Their mode of Action: Antineoplastic Agents: Cancer chemotherapy, role of alkylating agents and antimetabolites in treatment of cancer. Biological action of mechlorethamine, cyclophosphamide, melphalan, uracil,and 6-mercaptopurine.
Cardiovascular Drugs: Biological action of methyldopa, propranolol, amyl nitrate, verapamil, Atenolol.
Antihistaminic agents: Ethylene diamine derivatives, amino alkyl ether analogues, cyclic basic chain analogues.
Antifertility agents: General antifertility agents. HIV and anti AIDS drugs,
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, et al.
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 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.

Course Outcomes:
CO1: Demonstrate understanding of the basic principles of drug design and drug action.
CO2: Apply the knowledge of pharmacokinetics and pharmacodynamics in drug design.
CO3: Understand the SAR and mode of action of antibiotics.
CO4: Know the neurotransmitters SAR and their mode of action.
CO5: Analyze the SAR and mode of action of some antineoplastic, cardiovascular, antihistaminic, antifertility and diuretics agents.

SEMESTER-IV
CHEM 408
Organic Chemistry Special Theory -5
(Polymer Chemistry)

Lectures: 60
Max. Marks: 80

Course Objectives: The main objective of this course is to understand the fundamental concepts of polymerization. To know about various types of polymerization reaction and their mechanisms. To learn the various techniques of polymer synthesis and polymer characterization. To know various applications of biodegradable polymers.

Note: *Ten questions will be set by the examiner selecting **TWO** from each unit. As far as possible every question will be divided into **Two – Three Parts**. The students shall attempt **FIVE** questions selecting **ONE** from each unit.*

UNIT -I
Chemistry of Polymerization: Macromolecular Concept, Chain polymerization – Radical, Cationic and Anionic polymerization, Step Growth polymerization, Co-ordination polymerization, Kinetics of chain and step growth polymerization. Concept of chain transfer, Concept of copolymerization, Graft and Block copolymers, Copolymer equation, Monomer reactivity ratio, Alfrey-price scheme.

UNIT- II
Polymer synthesis: Bulk, solution, suspension, polycondensation, interfacial condensation and emulsion techniques of polymer synthesis
Polymer Characterization: Average molecular weight concept. Number, weight and viscosity, average molecular weights, Polydispersity and molecular weight distribution, The practical significance of molecular weight. Measurement of molecular weights - End group, viscosity, light scattering, osmotic and ultra centrifugation methods. Analysis and testing of polymers - Chemical analysis, Spectroscopic methods, Thermal Analysis, XRD and SEM.

Unit III
Stereoisomerism in polymers: Types of stereoisomerism in polymers, Monosubstituted ethylenes (Site of steric isomerism, Tacticity), Disubstituted ethylenes (1,1-disubstituted ethylenes, 1,2- disubstituted ethylenes), Stereoregular polymers: Significance of stereo-regularity (isotactic, syndiotactic, and atactic polypropenes), Cis- and trans-1,4-poly-1,3-dienes, Cellulose and amylose.
Morphology and order in crystalline polymers: Configuration of polymer chains. Crystal structures of polymers, Strain-induced morphology, Crystallization and melting, Polymer structures and physical properties - crystalline melting point, Tm, Effect of chain flexibility and other steric factors, entropy and heat of fusion, Glass transition temperature, Tg, Relationship between Tm and Tg, Effect of molecular weight, diluents, chemical structure, chain topology, branching and crosslinking on polymer properties.

UNIT- IV
Polymer Reactions: General introduction to the polymer reactions, Vulcanization, Chemical and radiation crosslinking, Graft co-polymerization, Methods of Graft Copolymerization. Polymer as carriers or supports, polymeric reagents, polymeric substrates, Merrifield resins.

UNIT-V
Commercial and Specialty Polymers: Applications of polyethylene, polyvinyl chloride, polyamides, polyesters, polyurethanes, phenolic and epoxy resins and Silicone polymers. Applications of starch, gelatin, pectin and chitosan in polymer industry. Biodegradable polymers (lactic and glycolic acid). Biomedical applications of polymers.

Books Recommended:

1. Molecular Mechanics, U. Burkert and N.L. Allinger, ACS Monograph 177, 1982.
2. Organic Chemist's Book of Orbitals. L. Salem and W.L. Jorgensen, Academic press.
3. Mechanism and Theory in Organic Chemistry, T.H.Lowry and K.C. Richardson, Harper and Row.
4. Introduction to Theoretical Organic Chemistry and Molecular Modeling, W.B. Smith, VCH,
5. Physical Organic Chemistry, N.S. Isaacs, ELBS/Longman.
6. Supramolecular Chemistry; Concepts and Perspectives, J.M. Lehn, VCH.
7. The Physical Basis of Organic Chemistry, H.Maskill, Oxford Univ. Press.
8. Textbook of Polymer Science, F.W. Billmeyer Jr. Wiley.
9. Polymer Science, V.R. Gowarikar, N.V. Visvanathan and J. Sreedhar, Wiley Eastern.
10. Functional Monomers & Polymers, K. Takemoto, Y. Inaki and R.M. Ottanbrite.
11. Contemporary Polymer Chemistry, H.R. Alcock and F.W. Lambe, Prentice Hall.
12. Physics & Chemistry of Polymers, J.M.G. Cowie, Blakie Academic and Professional.

Course Outcomes:
CO1: Apply the basic concepts of polymerization reactions in polymer synthesis.
CO2: Understand the various techniques of polymer synthesis and characterization.
CO3: Explain the stereoisomerism and its effect on polymer structures and physical properties
CO4: Understand the importance of polymer as carriers, reagents and polymeric substrates in polymer applications.
CO5: Compare the applications of various natural and synthetic polymers.

SEMESTER-IV
CHEM 409
Physical Chemistry Special Theory-2
(Quantum Chemistry)

Lectures:60
Max. Marks:80

COURSE OBJECRTIVES: This course is introduced to impart students with the knowledge of various theories for non – degenerate states, quantum mechanical treatments of molecular systems and Huckel Molecular Orbital Theory of conjugated π - electron Systems.

NOTE: *Ten questions will be set by the examiner selecting TWO from each unit. As far as possible, each question will be sub-divided into two – Three parts. The student shall attempt FIVE questions in total, selecting ONE question from each unit.*

UNIT-I
Time-independent perturbation theory for non-degenerate states. 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. First order perturbation for degenerate states. Effect of perturbation on ground and excited state hydrogen atom (Stark effect).

UNIT-II
Variation theory for ground and excited state energy and wave function. Linear and non-linear variation functions. Application of variation method to ground stae helium atom, hydrogen atom, one dimensional harmonic oscillator and particle in one dimensional box. Basic concept of Hellmann-Feynman theorm.

UNIT-III
Many -Electron Atoms: Concept of spin and Pauli exclusion principle. Slater determinants. Hartree Self Consistent –Field Method and Hartree –Fock Self Consistent –Field Method. Electron correlation and configuration interaction. Condon-Slater rules. Concept of Koopman's theorm.

UNIT-IV
Quantum Mechanical Treatments of Molecular Systems: The Born-Oppenheimer Approximation. The linear combination of atomic orbital (LCAO)-approximation. Molecular orbital and Valence –Bond treatments with respect to H_2 and H_2^+. Basic concept of Density Functional Theory

UNIT-V
Huckel Molecular Orbital Theory of conjugated π - electron Systems (conjugated linear and cyclic hydrocarbon systems). Application to ethylene, allyl systems (radical, cation and anion), Butadiene, cyclobutadiene and benzene and their physical representations.

Books Recommended:
1. Quantum Chemistry: An Introduction By H.L. Strauss
2. Quantum Chemistry By D.A. McQuarri
3. Quantum Chemistry By I.N. Levine
4. Molecular Quantum Chemistry By P.W. Atkin
5. Fundamental of Quantum Chemistry By T.E. Peacock
6. Elementary Quantum Chemistry By F.L. Pilar

By the end of the course, students will be able to
CO1: derive expressions for wave function and energy of a particle in one dimensional box
CO2: apply variation method to ground state helium and hydrogen atom
CO3: solve problems by using suitable expressions and equations of quantum chemistry
CO4: understand the quantum mechanical treatment of molecular systems
CO5: know about the various theories and laws of conjugated π - electron Systems
CO6: apply Huckel Molecular Orbital theory to different conjugated systems

SEMESTER-IV
CHEM 410
Physical Chemistry Special Theory-3
(Solid State Chemistry)

Lectures: 60
Max. Marks: 80

COURSE OBJECRTIVES: This course is introduced to impart students with the knowledge of crystal structure, various properties of crystals and bonding in crystals. This course will also impart knowledge and understanding of superconductivity phenomenon and solid-state reactions.

Note: *Ten questions will be set by the examiner selecting **TWO** from each unit. As far as possible, every question will be divided into **Two – Three Parts**. The students shall attempt **FIVE** questions selecting **ONE** from each unit.*

UNIT - I

X-ray Diffraction & Crystal Structure: X-rays Diffraction by crystals. The Laue equations and Bragg's law. Definitions related to crystal structure. Crystallographic direction and crystallographic phases. X-ray diffraction experiments: The powder method and the single crystal method. Reciprocal lattice. Structure factor and its relation to intensity and Electron density.

UNIT - II

Bonding in crystals: Ionic crystals, lattice energy of ionic crystals, metallic crystals. Band theory. Imperfections: Point defects (Schottky and Frankel defects). Thermodynamic derivation of these defects. Theories of Bonding: Free electro theory (a qualitative treatment) Zone theory; allowed energy zones ,Brillioun zones, k – space, Fermi surfaces and density states.

UNIT - 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: Dielectric properties: Piezoelectricity, Ferro electricity, Ionic conductivity and electric breakdown.

UNIT – IV

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

UNIT - V

Solid State Reactions: General principles: experimental procedures, kinetics of solid state reactions, vapour phase transport methods, interaction or ion exchange reaction, electrochemical reduction methods, preparation of thin films, growth of single crystal.

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

By the end of the course, students will be able to

CO1: analyse the structure and properties of crystals
CO2: know the bonding pattern and defects in solids
CO3: solve problems by using suitable expressions and equations of crystals structures
CO4: understand various theories of superconductivity
CO5: know about the various solid state reactions
CO6: develop and synthesise thin film and single crystal

SEMESTER-IV
CHEM 411
Physical Chemistry Special Theory-4
(Biophysical Chemistry)

Lectures: 60
Max. Marks: 80

COURSE OBJECRTIVES: This course is introduced to impart students with the knowledge of cell membrane and its structure, crystal structure, statistical mechanics in biopolymers and different mechanism of membrane transport. This course will also impart knowledge and understanding of biomolecular interactions and sequence and structure of protein molecules.

Note: *Ten questions will be set by the examiner selecting **TWO** from each unit. As far as possible, every question will be divided into **Two – Three Parts**. The students shall attempt **FIVE** questions selecting **ONE** from each unit.*

UNIT – I
Cell membrane and its structure: The Cell Membrane, 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.

UNIT – II
Statistical mechanics in biopolymers chain configuration of macromolecules, statistical distribution end – to - end dimensions, Polypeptide and protein structures and protein folding. calculation of average dimensions for various chain structures. Neurobiophysics: neurons, synapse, physics of membrane potential,neurotransmitters: Serotonin, GABA.

UNIT – III
Mechanism of Membrane Transport: Transport through cell membrane, active and passive transport (chemi-osmotic theory) systems, 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.

UNIT – IV
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.

UNIT –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 heamoglobin and myoglobin and their physiological roles, Protein folding and refolding, Protein misfolding, Chaperones and chemical factors (Intra and intermolecular interactions) leading to folding/refolding/misfolding. Brain diseases associated with it, structure of virus.

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 : VasanthaPattabhi, N.Gautam
10. Biophysical Chemistry: Gurtu&Gurtu

By the end of the course, students will be able to
CO1: know about the cell membrane and its structure and thermodynamic considerations
CO2: understand mechanism of membrane Transport phenomenon
CO3: solve problems by using suitable expressions and equations of crystals structures
CO4: explain miomolecular Interactionsbetween biomolecules
CO5: understand sequence and structure of protein and other biomolecules

SEMESTER-IV
CHEM 412
Physical Chemistry Special Theory-5
(Chemistry of Macromolecules)

Lectures: 60
Max. Marks: 80

COURSE OBJECRTIVES: This course is introduced to impart students with the knowledge of macromolecules including their thermodynamics and crystallinity. This course will also impart knowledge and understanding of mechanical properties of polymers, flow behaviour of polymer fluids along with their kinetics.

Note: *Ten questions will be set by the examiner selecting* ***TWO*** *from each unit. As far as possible, every question will be divided into* ***Two – Three Parts****. The students shall attempt* ***FIVE*** *questions selecting* ***ONE*** *from each unit.*

UNIT – I
Introduction to Macromolecules: Introduction, classification and importance of macromolecules, synthetic and natural polymers, polymerization (condensation and addition reactions), 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.

UNIT – II
Thermodynamics of Polymer solutions: Introduction and Criteria for polymer solubility, the Flory – Huggins Theory (changes in enthalpy, entropy, free energy and chemical potentials of mixing), determination of interaction parameter; θ temperature and cloud point, strengths and weaknesses of the Flory – Huggins Theory, concept of free volume theories, Flory-Krigbaum theory for dilute polymer solutions.

UNIT – III
Polymer Crystallization and Molecular weights determination: Introduction, configuration and crystallinity of polymer materials, energetics of phase change: homogeneous and heterogeneous nucleations, polymer bends and crystallization of miscible blends, melting of crystals, polymers with liquid crystal order, histogram of the degree of polymerization, molecular weight determination by Osmometry, light scattering, ultracentrifugation, intrinsic viscosity and gel permeation chromatography.

UNIT – IV
Mechanical Properties of Polymers and flow behaviour of polymer fluids:
Introduction, stress-strain behaviour and influence of molecular weight and temperature, the glassy transition temperature, polymer fracture and fatigue failure. Steady shear viscosity of polymer fluids (qualitative behaviour), theory of shear viscosity, viscometric flow (capillary viscometer) and kinetic theory of rubber elasticity.

Unit-V
Polymerization Kinetics:
Chain growth polymerization: Radical polymerization, kinetic model of radical polymerization and its verification, equilibrium of radical polymerization and temperature effect in radical polymerization. Ionic polymerization (cationic and anionic), kinetics of Ziegler – Natta catalysis in stereoregular polymerization (only qualitative discussion), step – growth polymerization., kinetics using equal reactivity hypothesis and equilibrium step-growth polymerization.

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
8. Fundamental of Polymers:Prof. Anil Kumar, R.K.Gupta, McGraw-Hill Publications

By the end of the course, students will be able to
CO1: know about the classification and thermodynamics of themacromolecules
CO2: apply different methods of molecular mass determination of polymers
CO3: explain the mechanical properties and flow behaviour of polymers
CO4: understand the kinetics of polymerisation

SEMESTER IV
CHEM 413
Inorganic Chemistry Special Practical -1

Max. Marks – 100

Course Objectives: This course aims at to provide the students with the opportunity to develop experimental skills by exposing them to work independently with instruments and will be allowed to explore various synthetic protocols in inorganic synthesis followed by preparation of database and also to be able to check the correctness of the results Very important course work aiming at developing analytical and synthetic skills finding use both in research and industry.

Preparation of the following compounds and a study of the important properties *viz*. Molar conductance, magnetic susceptibility, electronic and infrared spectra. 1. Stannic iodide, 2. Bis(acetylacetonato) oxovanadium (IV), 3. Mercuration of phenol, 4. Hexa ammine nickel (II) chloride. 5. Lead tetraacetate, 6. Cis- and trans- $[Co(en)_2Cl_2]Cl$

INSTRUMENTAL ANALYSIS:
A) Conductometric Titrations:
i) Differential behaviour of acetic acid to determine the relative acid strength of various acids.
ii) Strong acid-strong base titration in acetic acid.
iii) Potassium acetate- pyridine titration in acetic acid.
B) Potentiometric Titration:. 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, ii) Chloride-Iodide mixture.
C) **Colorimetric Analysis:**
1) Verification of Beer's law for KMnO4, K2Cr2O7 solutions and determination of the conc. of KMnO4, K2Cr2O7.
2) Colorimetric determination of Iron (II) with o-Phenanthroline method.
3) Determination of traces of manganese (in steel samples) colorometrically by oxidation to permanganic acid with potassium periodate.
4) Spectrophotometric determination of pK value of an indicator (acid dissociation constt. of methyl red)
5) Simultaneous determination of chromium (as $Cr_2O_7^{2-}$) and manganese (as MnO_4^-) in mixture.
6) Simultaneous determination of Fe(II) and Fe(III).
7) Photometric titration (simple illustrations)
8) Determination of stability constant of a complex by spectrophotometric method.
(D) pH metric –titrations
1) Acid base titrations.
2) Mixtures of acids with a base.
E) Polarography/Pulse polarography:
1) Determination of half wave potentials of cadmium, zinc and manganous ions in potassium chloride solution.
2) Investigation of the influence of dissolved oxygen.
3) Differential pulse polarographic determination of copper and zinc.
4) Determination of formation constant of a complex metal ion by polarography/pulse polarography.
(F) Cyclic voltammetry:
1. Determination of E^o and n values of $[Fe(CN)_6]^{3-}$/ $[Fe(CN)_6]^{4-}$ couple.
2. Study of electrode mechanism of cyclic voltammetry.
(G) Flame Photometry: Determination of sodium, potassium and calcium

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.

Course Outcomes:
CO 1:Understand various synthetic techniques to prepare inorganic complexes.
CO2: Explain the characterization by inorganic complexes with elemental analysis and spectral techniques.
CO 3:Apply the fundamentals of conductometric, potentiometric and pH metric titrations for analysis of given sample solutions.
CO 4:Apply the fundamentals of spectrophotometric, voltammetric and polarographic techniques for quality control.
CO 5:Learn data handling and analysis and also to develop problem solving ability.

SEMESTER – IV
CHEM 414
Organic Chemistry Special Practical-1

Max. Marks: 100

Course Objectives: The objective of this course is to provide the practical knowledge of the isolation of active component from natural sources and to know the concept of stepwise synthesis. To be acquainted with various combinations of reactions that can be exploited to form a product and to have experience to work under different reaction conditions.

Extraction of Organic Compounds from Natural Sources: Isolation of Caffeine from tea leaves, casein from milk (the students are required to try some typical color reactions of proteins), lactose from milk (purity of sugar should be checked by TLC and PC and R_f value reported). Isolation of diosgenin from Fenugreek seeds (Methi seeds), lycopene from tomatoes and β- carotene from carrots.
Multistep Synthesis: Synthesis of Vacor or vacor type compound, Synthesis of Indigo etc,
Synthesis of polymers, Preparation of polyacrylamide from acrylamide, Preparation of polyacrylic acid from acrylic acid. and Any other reaction as per requirement.
TLC and Paper Chromatography: Separation and identification of the sugars present in the given mixture of glucose, fructose and sucrose by paper chromatography and determination of R_f values.
Spectroscopy: Identification of some organic compounds by the analysis of their spectral data (UV, IR, PMR, CMR and MS)
All the students must submit the recrystallised product along with yield, melting point and Rf value of the compounds for all the stages of preparation.

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.
6. Laboratory Experiments in Organic Chemistry, R. Adams, J. R. Johnson and C. F. Wilcox. The Macmillan Limited, London.

Course Outcomes:
CO1: Apply the knowledge of basis procedure of isolation for the isolation of active component from natural sources.
CO2: Understand the concept of multistep synthesis under different reaction conditions.
CO3: Develop the ability to compile interpreted information in the form of lab record.
CO4: Able to interpret the structure of synthesized organic compound by applying the spectroscopic techniques.
CO5: Know about how to defend viva-voce.

SEMESTER IV
CHEM 415
Physical Chemistry Special Practical - 1

Max. Marks – 100

COURSE OBJECTIVES: This course is introduced to impart knowledge of various experimental methods and techniques used for the determination of viscosity of solutions and Walden's product. This course will also impart knowledge and understanding of various potentiometric titrations, flame photometric measurements, colorimetry and polarimetry measurements.

1. **Viscosity Measurements:** Verification of the Jones – Dole equation for simple electrolytes in water and in aqueous mixtures of organic solvents.
2. **Conductometric Measurements:** Determination of Walden's product in case of simple electrolytes.
3. **Potentiometric Titration:** Titration of HCl with NaOH, determination of dissociation constant of acetic acid and phosphoric acid. Oxidation – reduction titration.
4. **Flamephotometric Measurements:** Estimation of concentration of Ca^{+2}, Na^{+} and K^{+} ions and in the given aqueous solution at ppm level.
5. **Determination of Molar Mass:** (i) Cryoscopic and Rasts's methods.
6. **Colorimetry Measurements:** Determination of composition and free energy of formation of ferric ions – salicylic acid complex using Job's continuous method.
7. **Polarimetry Measurements:** Determination of specific and molecular rotation, percentage of tow optically active substances, kinetics of acid catalysed inversion of cane sugar and comparison of strengths of two acids.

Books Recommended:

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

By the end of the course, students will be able to

CO1: understand the safe handling of chemicals and safety measures to be followed during the laboratory
CO2: verify Jones-Dole equation by using viscosity measurements
CO3: determine Walden's Product using conductance of simple electrolytes in water
CO4: estimate the concentration of Ca^{+2}, Na^{+} and K^{+} ions and in the given aqueous solution by using flame photometric measurements.
CO5: Determine composition and free energy of formation of ferric ions – salicylic acid complex using Job's continuous method
CO6: Determine specific and molecular rotation of optically active substances,
CO7: analyse the kinetics of acid catalysed inversion of cane sugar and comparison of strengths of two acids.

SEMESTER - IV

CHEM 416
(SEMINARS)
FOR ALL THREE SPECIALIZATIONS

Time: ½ hr
Max. Marks: 25x2=50

Every candidate will have to deliver a seminar of 20-30 minutes duration on a topic (not from the syllabus) 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 specializations) 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) Content
(ii) Expression
(iii) Presentation
(iv) Depth of the subject matter and answers to the questions.