MAHARASHTRA EDUCATION SOCIETY

ABASAHEB GARWARE COLLEGE

(Autonomous)

(Affiliated to Savitribai Phule Pune University)

Two Year M.Sc. Degree Program in Chemistry
(Faculty of Science and Technology)

Syllabi under Autonomy
M.Sc. I (Chemistry)

Choice Based Credit System Syllabus
To be implemented from Academic Year 2022-2023

Title of the Course: M. Sc. (Chemistry)

Preamble:

Taking into consideration the rapid changes in science and technology and new approaches in different areas of Chemistry and related subjects, Board of studies in Chemistry after a thorough discussion with the teachers of Chemistry from Abasaheb Garware College and experts from industry as well as other Academic institutions has prepared the syllabus of M.Sc. I Semester - I and Semester- II (w.e.f. 2022-23) Chemistry course under the Choice Based Credit System (CBCS). The model curriculum as developed by U. G. C. is used as a guideline for the present syllabus.

Program Outcomes:

1. To impart knowledge of Chemistry covering all the aspects viz. physical, inorganic, organic and general Chemistry

2. To provide laboratory experience to the students by performing experiments based on topics taught in theory

3. Create awareness and sense of responsibilities towards environment and apply knowledge to solve the issues related to Environmental pollution.

4. Apply knowledge to build up small scale industry for developing endogenous product.

5. Apply various aspects of chemistry in natural products isolations, pharmaceuticals, dyes, textiles, polymers, petroleum products, forensic etc. and also to develop interdisciplinary approach of the subject

Eligibility:

Passed B.Sc. Chemistry or equivalent course.

Structure of the Course: M.Sc. Chemistry

Year	Semester	Course Type	Course Code	Course Title	Remark	Credit	No. of Lectures /Practical to be conducted
1	I	Compulsory	PSCH-111	Physical Chemistry-I (Fundamentals of Physical Chemistry)	Theory	04	60
		Compulsory	PSCH-112	Inorganic Chemistry-I (Molecular Symmetry and Chemistry of Main Group Elements)	Theory	04	60
		Compulsory	PSCH-113	Organic Chemistry-I (Basic Organic Chemistry)	Theory	04	60
		Elective	PSCHELE-114	**Section-I:** General Chemistry-I, **A**: Introduction to Solid State of Matter **B**: Mathematics for Chemists **C:** Introduction to Chemical Biology-I	Theory (Select any one option)	02	30
			PSCHPELE-114	**Section-II: General Chemistry Practical** **A:** Inorganic Chemistry-Material Analysis, Synthesis and Applications **B:** Chemical Biology Practical-I	Practical (Select any one)	02	A:11 or B:11
		Compulsory	PSCHP-115	Basic Practical Chemistry-I	Practical	04	22
	II	Compulsory	PSCH-121	Physical Chemistry - II (Molecular Spectroscopy and Nuclear Chemistry)	Theory	04	60
		Compulsory	PSCH-122	Inorganic Chemistry - II (Coordination and	Theory	04	60

				Bioinorganic Chemistry)			
		Compulsory	PSCH-123	Organic Chemistry-II (Photochemistry, Pericyclic and Organic spectroscopy)	Theory	04	60
		Elective	PSCHELE-124	**Section-I:** General Chemistry-II **A**:Material Characterization Technique **B**: Organometallic and Inorganic Reaction Mechanism **C:** Introduction to Chemical Biology-II	Theory (Select any one option)	02	30
			PSCHPELE-124	**Section-II: General Chemistry, Practical** **A**: Electroanalytical Techniques of Analysis **B**: Chemical Biology Practical-II	Practical (Select any one option)	02	A:11 or B: 11
		Compulsory	PSCHP-125	Basic Practical Chemistry-II	Practical	04	22

M. Sc.-II: Organic Chemistry

Year	Semester	Course Type	Course Code	Course Title	Remark	Credit	No. of Lectures /Practical to be conducted
2	**III**	Compulsory	PSCHO-231	Organic Reaction Mechanism and Biogenesis	Theory	04	60
		Compulsory	PSCHO-232	Structure Determination of Organic Compounds by Spectroscopic Methods	Theory	04	60
		Compulsory	PSCHO-233	Stereochemistry and Asymmetric Synthesis of Organic Compounds.	Theory	04	60

		Elective	PSCHOELE-234	**A)** Protection - De-protection, Chiron approach and Carbohydrate Chemistry **B)** Designing Organic Syntheses and Heterocyclic Chemistry	Theory (Select any one)	04	60
		Compulsory	PSCHOP- 235	Solvent Free Organic Synthesis	Practical -I	04	24
	IV	Compulsory	PSCHO-241	Chemistry of Natural Products	Theory	04	60
		Compulsory	PSCHO-242	Organometallic Reagents in Organic Synthesis	Theory	04	60
		Elective	PSCHOELE-243	**A)** Medicinal Chemistry **B)** Applied Organic Chemistry	Theory (Select any one)	04	60
		Compulsory	PSCHOP-244	Convergent and divergent Organic Syntheses.	Practical -II	04	24
		Elective	PSCHOPELE-245	**A:** Ternary Mixture Separation **B:** Carbohydrates Synthesis and Isolation of Natural Products **C:** Project / Industrial Training/ Internships/ Summer Project	Practical -III (Select any two)	04	A: 12 B: 12

M. Sc.-II : Analytical Chemistry

Year	Semester	Course Type	Course Code	Course Title	Remark	Credit	No. of Lectures /Practical to be conducted
2	**III**	Compulsory	PSCHA-231	Electrochemical and Thermogravimetric Methods of chemical analysis	Theory	04	60
		Compulsory	PSCHA-232	Analytical Method Development and Extraction Techniques	Theory	04	60
		Compulsory	PSCHA-233	Advanced Chromatographic	Theory	04	60

				Methods of Chemical Analysis			
		Elective	PSCHAELE-234	**A)** Bioanalytical Chemistry **B)** Analysis of Food and Controlled Substances	Theory (Select any one)	04	60
		Compulsory	PSCHAP-235	Basics of Instrumental Methods of Chemical Analysis	Practical -I	04	24
	IV	Compulsory	PSCHA-241	Advanced Analytical Spectroscopic Techniques	Theory	04	60
		Compulsory	PSCHA-242	Chemical Methods of Pharmaceuticals Analysis	Theory	04	60
		Elective	PSCHAELE-243	**A)** Laboratory Automation and Environmental Analytical Chemistry Or **B)** Analytical Chemistry of agriculture, polymer and Detergents	Theory (Select any one)	04	60
		Compulsory	PSCHAP-244	Applied Analytical Chemistry Practical	Practical -II	04	24
		Elective	PSCHAPELE-245	**A)** Optional Analytical Chemistry Practical Or **B)** Project Products	Practical -III (Select any one)	04	24

Semester-I

Course code and Title: PSCH-111, Physical Chemistry-I

(Fundamentals of Physical Chemistry) **Lectures: 60 (Credits-4)**

SECTION - I (2 Credits, 30 Hours)

Learning outcomes:

1. Student should visualize/ imagine molecules in 3 dimensions.
2. To understand the concept of symmetry and able to pass various symmetry elements through the molecule.
3. Understand the concept and point group and apply it to molecules.
4. To understand product of symmetry operations.
5. To apply the concept of point group for determining optical activity and dipole moment.
6. Student should understand the importance of Orthogonality Theorem.
7. They should able to learn the rules for constructing character table.
8. Using reduction formulae should be able to find out the possible type of hybridization.
9. Student should know the concept of SALC.
10. Student able to find out character for reducible representation.
11. To know about projection operator.
12. Apply projection operator to find out the normalized wave function for atomic orbital.
13. Student should correlate the application of symmetry to spectroscopy.
14. Students able to find out the possible modes of vibration.
15. From the previous knowledge of symmetry student must able to find out which mode are IR active.

1. Thermodynamics (06 Hours)

State function, path function, exact differential and inexact differential, internal energy and enthalpy, temperature dependent internal energy and enthalpy, reversible and irreversible adiabatic expansion. The entropy of irreversible changes, the Helmholtz and Gibbs function, Entropy and entropy change in an ideal gas with temperature and pressure, Clausius inequality, chemical potential, chemical potential of a substance in a mixture.

2. Change of State (06 Hours)

Partial molar quantities, methods for determination of molar quantities, ideal solutions, Raoult's and Henery's law, Thermodynamics of Gibbs function of mixing, colligative properties: Elevation in boiling point, depression in freezing point and osmosis.

3. Molecular Thermodynamics (10 Hours)

Molecular energy levels, Boltzmann distribution law, partition functions and ensembles, translational, rotational and vibrational partition function of diatomic molecule, obtaining

energy, heat capacity, entropy and equilibrium constants from partition functions, Maxwell-Boltzmann, Fermi-Dirac and Bose-Einstein statistics.

4. Chemical Bonding **(08 Hours)**

Valence bond theory, hybrid orbitals, geometry and hybridization, molecular orbital theory for di and tri atomic molecule, linear variation method, approximations underlying Huckel theory, applications to simple π-systems.

SECTION – II (2 Credits, 30 Hours)

Chemical Kinetics and Reaction Dynamics

1. Rate Laws **(07 Hours)**

Recapitulations of basic concept, the temperature dependent reaction rates, reaction moving towards equilibrium, consecutive reaction, parallel reactions, pre-equilibria, unimolecular reactions.

2. Kinetics of Complex Reactions **(04 Hours)**

Fast reactions: flash photolysis, flow technique, stopped flow technique, relaxation method, the steady state approximation, chain reactions - free radical polymerization reaction between H_2 and Br_2, explosive reaction.

3. Molecular Reaction Dynamics **(06 Hours)**

Collision theory of bimolecular gas phase reactions, diffusion controlled and activation controlled reaction in solution, activated complex theory of reaction rate, Eyrings equation

4. Enzyme Catalysis **(05 Hours)**

Michaelis mechanism, effect of pH and temperature on enzyme catalyzed reactions, limiting rate, Lineweaver, burk and Eadie equation and plots, inhibition of enzyme action, competitive inhibition and non- competitive inhibition.

5. Quantum Chemistry **(08 Hours)**

Applications of quantum chemistry- blackbody radiation, photoelectric effect, de Broglie hypothesis and uncertainty principle and its experimental evidence. Schrödinger wave equation, particle in one dimensional box, Normalization and orthogonality of wave function, particle in three dimensional box, hydrogen like atoms (no derivation).

References:

1. Physical Chemistry by P.W. Atkins and De Paul
2. Physical Chemistry by T. Engel and P. Reid
3. Physical Chemistry for biological sciences by Raymond Chang (Universal books, 2000)
4. Physical Chemistry by Marron and C. F. Prutton
5. Physical Chemistry by G.M. Barrow

6. Quantum Chemistry by I. Levine
7. Quantum Chemistry by R.K. Prasad
8. Fundamentals of Quantum Chemistry 2nd Ed. James E. House

Course code and Title: PSCH-112, Inorganic Chemistry-I (Molecular Symmetry and Chemistry of Main Group Elements)

Lectures: 60 (Credits-4)

SECTION-I (2Credits, 30 Hours)

Molecular Symmetry and its Applications

1) Molecular Symmetry and Symmetry Groups (12 Hours)

Symmetry elements and operations, Symmetry planes and reflections, the inversion centre, proper axes and proper rotations, improper axes and improper rotation, products of symmetry operations, equivalent symmetry elements and equivalent atoms, general relations among symmetry elements and symmetry operations, classes of symmetry operations, symmetry elements and optical isomerism, symmetry point groups, classification of molecular point groups. Defining properties of a group, group multiplication table, some examples of group, subgroups and classes.

2) Representations of Groups (08 Hours)

Matrix representation and matrix notation for geometric transformation, The Great Orthogonality Theorem and its consequence, character tables (No mathematical part),wave function as basis for irreducible representations.

3) Symmetry Adapted Linear Combinations (05 Hours)

Projection operators and their use of construct SALC (Construction of SALC for sigma bonding for molecules belonging point groups: D_{2h}, D_{3h} D_{4h}, C_{4v}, Td., Oh., normalization of SALC, transformation properties of atomic orbital, MO's for sigma bonding,ABn molecules, tetrahedral AB_4 and Oh AB_6 cases.

4) Application of Group theory to Infrared Spectroscopy and Raman Spectroscopy

(05 Hours)

Introduction, selection rules, polyatomic molecules, possible vibrations in a linear molecule, bending modes, symmetry of vibrations and their IR activity, Group vibration concept and its limitations, IR spectra related to symmetry of some compounds, IR spectra of complex compounds. Raman spectra of diamond, ammonia

References:

1)Chemical Applications of Group Theory by F. A. Cotton
2)Symmetry and spectroscopy of molecules by K. VeeraReddy
3)Group Theory and its Chemical Application, P.K. Bhattarchrya
4) Inorganic Chemistry by Shriver and Atkins

5)Concise Inorganic Chemistry by J. D. Lee
6) Inorganic chemistry: principle of structures and reactivity by Huheey, Keiter, Medhi

Section-II (2 Credits, 30 Hours)

Chemistry of Main Group Elements

1) Hydrogen and its compounds: (02 Hours)

Classification of Hydrides, electron deficient, electron precise and electron rich hydrides.; PH_3, SbH_3, AsH_3, Selenides, Tellurides.

2) Alkali and Alkaline Earth Metals (03 Hours)

Solutions innon - aqueous media, application of crown ether in extraction of alkali and alkaline earth metal

3) Boron Group (04 Hours)

Boron Hydrides, preparation, structure and Bonding with reference to LUMO, HOMO, interconversion of lower and higher boranes, metalloboranes, carboranes, reactions of organoboranes, STYX rules and structure of higher boranes.

4) Carbon Group (04 Hours)

Allotropes of carbon, Diamond, Graphite, Graphene, fullerenes, carbon nanotube with synthesis, properties , Structure- single walled and multi walled and its application, Intercalation compounds of graphite, Silicates, including Zeolites.

5) Nitrogen Group (03 Hours)

Nitrogen activation, Boron nitride, Oxidation states of nitrogen and their inter conversion, PN and SN Compounds, Applications of PN and SN compounds

6) Oxygen Group (03 Hours)

Metal Selenides and Tellurides, oxyacid's, and oxoanions of Sulphur and nitrogen. Ring, Cage and Cluster compounds of p-block elements.

7) Halogen Group (02 Hours)

Interhalogens, pseudohalagen, Synthesis, Properties and Applications, Structure, Oxyacid's andOxyanions of Halogens.

8) Noble gases (02 Hours)

Occurrence**,** Compounds of Xenon-with fluorine and Oxygen and its uses

9) Nanomaterial (07 Hours)

a) Preparative methods: Chemical methods, Solvo thermal combustion synthesis, microwave, co-precipitation, Langmuir Blodgett (L-B) method, Biological method: synthesis using micro-organisms, ceramic, precursor method, sol-gel method (applications in biosensor), microwave synthesis.

b) Applications: semiconductor, solar cell, top down and bottom up approach, biosensor

References:

1) Inorganic Chemistry by Shriver and Atkins
2) Concise Inorganic Chemistry by J. D. Lee

3) Inorganic chemistry by Principle of Structures and Reactivity by Huheey, Keiter, Medhi
4) Inorganic Chemistry by Catherine Housecraft
5) Inorganic Chemistry by Meissler and Tarr
6) Organometallics by Christoph Elschenbroich
7) Organometallics by A Concise Introduction by Christoph Elschenbroich and Albrecht Salzer
8) Basic Organometallic Chemistry by B. D. Gupta and A. J. Elias
9) Nanotechnology By Dr. Shulbha Kulkarni.

Course code and Title: PSCH-113, Organic Chemistry-I

Lectures: 60 (Credits-4)

SECTION-I (2 Credits, 30 Hours)

Basic Organic Chemistry

Learning outcomes

1. To understand some fundamental aspects of organic chemistry, to learn the concept aromaticity, to understand the various types of aromaticity

2. To study heterocyclic compound containing one and two hetero atoms with their structure, synthesis and reactions.

3 Able to assign R and S to given molecules; understand stereoselective and stereospecific reactions; acquire knowledge on topicity.

4. To study structure, formation, stability and related name reaction of intermediates like Carbocation, Carbanion, Free Radical, Carbenes and nitrenes; Recognize neighboring group participation

5. To study rearrangement reaction with specific mechanism and migratory aptitude of different groups.

6. To learn the preparation and reactions of ylides.

7. To understands the basis of redox reaction; acquire knowledge about the reagents which causes selective oxidation / reduction in various compounds; learn the basic mechanism of oxidation / reduction in organic compounds.

1. Structure and Reactivity: (08 Hours)

Aromaticity: Benzenoid and non-benzenoid compounds, Huckel's rule, antiaromaticity, generations and reactions, homoaromaticity, Application to carbocyclic and heterocyclic systems, annulenes, azulenes, current concepts of aromaticity.

Self-Learning: Captodative effect

2. Principles of Stereochemistry (14 Hours)

a) Stereochemical principles, enantiomeric relationship, diastereomeric relationship, R/S, E/Z nomenclature in N, S, P containing compounds, Stereogenicity, stereospecific and stereoselective reactions, topicity.
b) Configurational and conformational isomerism in acyclic (allenes) and cyclic (biphenyls, Spiranes) compounds

Self-Learning: Assignment of R/S and E/Z configuration of cyclic and acyclic carbon compounds

3. Heterocyclic Chemistry **(08 Hours)**

Synthesis and reactivity of common heterocyclic compounds containing one heteroatom: Furan, Pyrrole, Thiophene, Indole, Pyridine and Quinoline.

Self-learning: Synthesis and reactivity of common heterocyclic compounds containing two heteroatoms (O, N, S) Pyrazole, Imidazole

SECTION-II (2 Credits, 30 Hours)

Learning outcomes
At the end of the course the students will know and recall the fundamental principles of organic chemistry that include chemical bonding, nomenclature, structural isomerism, stereochemistry, chemical reactions and mechanism.
1. They will understand the **c**riteria for aromaticity in nonbenzenoid molecules and other advanced polycyclic aromatics
2. Understand the chemistry of monocyclic heterocycles, nomenclature and reactions
3. Learn the concept stereochemistry and its importance; their rules and the concept of chirality
4. Understand the role of various reaction intermediates like carbocation, carbanion, carbenes, radicals, and nitrenes in organic reactions; concept of NGP
5. Able to describe mechanism of different rearrangement reactions. Appreciates the various steps involved in the molecular rearrangements.
6. Use synthetic reagent of oxidation and reduction for solving the problems

1. Structure, Stability and Reactions of Reactive Intermediates **(05 Hours)**
Carbocation, Carbanion, Free Radical, Carbenes and Nitrenes, Benzyne

2. Rearrangements **(10 Hours)**
Beckmann, Hofmann, Curtius, Schmidt, Wolff, Lossen, Bayer-villiger, Sommelet, Favorskii, Pinacol-pinacolone, Benzil-benzilic acid, Fries, Tiffeneau Demjanov, Wittig, Claisen rearrangement

3. Ylides: **(05 Hours)**

Phosphorous, Nitrogen and Sulphur ylides

4. Organic transformations using Oxidation and Reduction Reactions (10 Hours)

Oxidising reagents: CrO_3, PDC, PCC, $KMnO_4$, MnO_2, Swern, SeO_2, $Pb(OAc)_4$, Pd-C, RuO_4, OsO_4, m-CPBA, O_3,$NaIO_4$, HIO_4, TEMPO, IBX, CAN, Dess-Martin, DDQ

Reducing reagents: Hydroboration, Catalytic hydrogenation using Pt, Pd, Ni, Willkinsons catalyst, and Wolff-Kishner reduction, Birch, Clemenson, Rosenmund, $SnBu_3H$, reduction using $NaBH_4$, LAH and DIBAL-H

References:

1. Organic Chemistry–by J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford)
2. Advanced Organic Chemistry –by J. March 6th Edition
3. Advanced Organic Chemistry (Part A) –by A. Carey and R.J. Sundberg
4. A guidebook to mechanism in organic chemistry – Peter Sykes 6th Ed.
5. Stereochemistry of carbon compound-by E.L. Eliel
6. Stereochemistry of organic compound-by Nasipuri Modern Synthetic reactions- H.O. House
7. Organic Synthesis – M.B. Smith
9. Organic chemistry –by Cram, Hammond, Pine and Handrickson
10. Mechanism and structure in Organic Chemistry – E. S. Gould
11. Heterocyclic Chemistry- J A Joule and K Mills
12. Principles of modern heterocyclic chemistry- A Paquette
13. Name reactions in heterocyclic chemistry – by Jie Jack Lee

Course code and Title: PSCHELE– 114, General Chemistry-I

Lectures: 60 (Credits-4)

SECTION-I: Theory Course (2 Credits, 30 Hours)

(Any one option is to be selected by candidate)

Elective Option-A : Introduction to Solid State of Matter

Learning outcomes

At the end of course student will understand

1. Bonding in solids – band theory
2. Electronic conductivity
3. Semiconductors, photoconductivity
4. Non-stoichiometry, defects and types of defects in solids
5. Ionic conductivity and their applications
6. Superconductivity and theory of superconductivity
7. Method of synthesis of solids

1. Bonding in Solids and Electronic Properties (Ref-1, 4) **(06 Hours)**

Recollect the concepts: Crystalline solids, unit cell, and types of unit cells

Introduction, Bondingin Solids—Free Electron Theory, Electronic Conductivity, Bonding In Solids—Molecular Orbital Theory, Simple Metals, Semiconductors—Si And Ge, Photoconductivity, The *P-N* Junction—Field-Effect Transistors, Bands In Compounds—Gallium Arsenide, Bands In D-Block Compounds—Transition Metal Monoxides.

2. Defects and Non-Stoichiometry (Ref-1, 4) **(08 Hours)**

Introduction, point defects—an introduction, defects and their concentration, intrinsic defects, extrinsic defects the concentration of defects, ionic conductivity in solids, solid electrolytes, fast-ion conductors: oxygen ion conductors, fast-ion conductors: sodium ion conductors, Applications: 1) fuel cells, 2) sensors, 3) electrochromic devices, non-stoichiometric compounds, introduction, non-stoichiometry in wustite, the titanium monoxide structure.

3. Superconductivity (Ref-1, 4) **(06 Hours)**

Introduction, Discovery, The Magnetic Properties Of Superconductors, Josephson Effects, The Bcs Theory Of Superconductivity, High Temperature Superconductors, Theory Of High Tc Superconductors, Uses Of High Temperature Superconductors

4. Synthesis of Solids (Ref-2 and 3) **(10 Hours)**

Introduction, Common Reactions Employed in Synthesis, Soft-Chemistry Routes, Ceramic Methods, Decomposition of Precursor Compounds, Combustion Synthesis, Mechano-chemical and Sono-chemical methods, Soft Chemistry Routes(Ion Exchange Reactions, Use of Fluxes, Sol–Gel Synthesis, Electrochemical Methods, Hydrothermal, Solvothermal and Ionothermal Synthesis), Chemical Vapour Deposition and Atomic Layer Deposition, Procedures of synthesis of some nano-materials- Gold and Silver nanoparticles, CdS nanoparticles, ZnO, TiO2 and Fe2O3 nanoparticles and Porous Silica

References

Ref.-1: Elaine A. Moore, Lesley E. Smart - Solid State Chemistry - an Introduction. Third Ed. / Fourth Ed. CRC Press (2012)
Ref-2: C. N. R. Rao, Kanishka Biswas, Essentials of inorganic materials synthesis, Wiley, 2015
Ref-3: Nanotechnology: Principles and Practices, S. K. Kulkarni, Third Ed. Springer
Ref-4: Anthony R. West, Solid State Chemistry and its Applications Second Edition (Student Edition), Wiley.

Elective Option-B: Chemical Mathematics

1. Matrices and Determinants **(08 Hours)**

Metrices-Definition, Types, Operations (Addition, Subtraction, Multiplication), Inverse, Adjoint, transpose of matrix, Applications of metrices in chemistry, Solution of linear equations in chemistry, Determinants- Definition, Product of determinant, Minor, cofactors, Application of determinant in Molecular Orbital Theory

2. Derivatives **(09 Hours)**

Basic rules of differentiation, Addition Subtraction, multiplication, division, differentiation of function of function, function of power of function, parametric functions,
Maxima and minima
Exact inexact differentials in thermodynamics
Partial derivatives and their applications in deriving Maxwell relations
Applications of derivatives in chemical kinetics, photochemistry and radioactivity

3. Integration **(07 Hours)**

Rules f integration, Integration by substitution, Integration by parts, integration using partial functions

4. Data interpretation and representation **(06 Hours)**

Graphical representation of functions, (linear, exponential, logarithmic various methods required to present the data, plotting graphs using Microsoft excel

References:

1) Chemical Maths Book, E. Steiner, Oxford University Press (1996).
2) Maths For Chemists Vol. 1 and 2, Martin MCR Cockett and G. Doggett, Cambridge (2003).
3) Mathematical Preparation for Physical Chemistry, F. Daniels, McGraw Hill (1972)
4) Mathematics for chemists by Bhupinder Singh,Pragati Prakashan (2019)

Elective Option-C: Introduction to Chemical Biology-I

Learning Outcomes:

The goal of this course is to introduce students to fundamental concepts in Chemical Biology and methods of chemistry used to solve problems in molecular and cell biology. After completion of this course, successful students will:
1) Students will be able to explore new areas of research in both chemistry and allied fields of science and technology.
2) Students will be able to function as a member of an interdisciplinary problem solving team.
3) To impart the students thorough idea in the chemistry of carbohydrates, amino acids, proteins and nucleic acids etc.
4) Be able to describe the chemical basis for replication, transcription, translation and how each of these central processes can be expanded to include new chemical matter.
5) Develop skills to critically read the literature and effectively communicate research in a peer setting.

1. Overview of Biochemical Concepts **(04 Hours)**

Central dogma of cell biology, prokaryotes- eukaryotes and subcellular components, Overview of cell metabolism, Interdisciplinary approach, Biomolecules as potential drug targets

2. Chemistry of Biomembranes **(07 Hours)**

Structure, Functions and Composition, Fluid Mosaic Model by Singer and Nicholson, Properties of membrane, Transport of Ions (Na+, K+, H+, Ca2+, Cl-) and Molecules (Glucose, Amino acids, Proteins), transport across the membrane, Uniport, Symport, Antiport, Active and Passive facilitated transport, Exocytosis and Endocytosis (Pinocytosis, phagocytosis, receptor mediated endocytosis), Drug transport, Amphipathic nature and Significance of liposomes

3. Carbohydrates **(05 Hours)**

Classification, Structure and Properties, Derived sugars and their significance, Glycoproteins, glycolipids

4. Lipids **(05 Hours)**

Classification, Structure and Properties of lipids, Saponification number, Iodine number, Acid number, Rancidity of lipids, Lipoproteins

5. Amino Acids and Proteins **(09 Hours)**

Introduction, Classification of amino acids, Physico chemical properties, Optical properties, Peptide bond, Primary, Secondary, Tertiary and Quaternary structure of proteins, Protein - Ligand interactions, Denaturation of proteins, Oligopeptide synthesis, Concept of proteomics

References:

1. Principals of biochemistry, Albert Lehninger (CBS Publisher and Distributers Pvt. Delhi.
2. Harper's Biochemistry by R.K. Murray, D. I. Granner, P. A. Mayes, (Prentice Hall International Inc.) 3. Biochemistry by U. Satynarayana
4. Biochemistry by J. L. Jain
5. Biophysical Techniques by Upadhyaya Nath

Course code and Title: PSCHPELE-114

SECTION-II: Practical Course **Lectures: 30 (Credits-2)**

(Any one option to be selected by candidate)

Elective Option-A: Inorganic Material Analysis, Synthesis and Applications

Time allotted: One practical session of 4 hours per week for one semester

Part-I: Analysis (at least three of the following) (Ref. -1)

1. Determination of Silica and Manganese from pyrolusite ore.
2. Determination of Aluminum and Silica from Bauxite ore.
3. Determination of silica and iron from hematite ore.
4. Determination of copper and iron from Chalcopyrite ore.

Part-II: Alloy Analysis (at least three of the following) (Ref. -1)

5. Determination of tin and lead from solder alloy.
6. Determination of iron and chromium from stainless steel alloy.
7. Determination of copper and nickel from cupranickel alloy.

Part-III: Synthesis of solid state materials / nano-materials **(any three) (Ref- 2 and 3)**

8. Synthesis of ZnO from zinc oxalate - precursor method and determine band gap by absorption spectroscopy
9. Synthesis of TiO_2 $TiCl_4$ or Ti-Isopropoxide by Sol-gel method and determine bandgap by absorption spectroscopy
10. Synthesis of Fe_2O_3 nanoparticles sol-gel/coprecipitation/hydrothermal (any one method)
11. ZnO, TiO_2, Fe_2O_3 nanoparticles powder XRD, SEM, TEM (at least one spectral analysis should be done)
12. Synthesis of Silver nanoparticles by using plant extract and determine band gap by absorption spectroscopy.

Part-IV: Applications of Solid State Materials

13. Removal and kinetics of photocatalytic dyes, degradation (methylene blue) by ZnO or TiO_2 photocatalysis (Ref-2)
14. Study of adsorption of phosphate ion on alfa-Fe_2O_3 (Ref-2)

References:

1. Text book of Quantitative Analysis by A.I. Vogel $3^{ed}ed^{n}$ (1963).
2. Experimental Inorganic Chemistry by Mounir A. Malati, Horwood
3. Nanotechnology by S. K. Kulkarni

Examination Scheme:

1. The examination structure will be given before the commencement of examination.
2. 50% students will be assigned experiment on part-I or II while remaining – (analysis of any one component) 50% students will assigned experiment on part- III and IV.
3. Use of only university supplied procedure will be allowed at the time of examination.

Elective Option - B: Chemical Biology-I Practical

Time allotted: One practical Session of 4 hours per week for one semester

1. Statistical treatment of experimental data (calculation of mean and standard deviation for given data and least square method for calibration curve method) - Compulsory

Perform at least 10 Practical from the following

1. Preparation of biological buffers.
2. Qualitative analysis of carbohydrates
3. Qualitative analysis of Lipids
4. Qualitative analysis of amino acids
5. Paper chromatographic / TLC separation of mixture of amino acids and their detection
6. Paper chromatographic separation of mixture carbohydrates and their detection
7. Quantitative estimation of Glucose by dinitro salicylic acid by using calorimetric method
8. Quantitative estimation of proteins by Loawry's method
9. Kjeldahl method of Protein Determination
10. Saponification number of fats
11. Iodine value of oil
12. Isolation Quantitative estimation of DNA by Diphenyl amine method

13. Determination of Inorganic Phosphate in Biological Samples

References:

1. A reference book of biochemistry practicals by Sadashivam
2. Practical approach to biochemistry by Plummer
3. Martin Holtzhauer, Basic Methods for the Biochemical Lab, First Edition, Springer

Examination Scheme:

1. The examination structure will be given before the commencement of examination.
2. Use of only supplied procedure will be allowed at the time of examination.

Course code and Title: PSCHP-115: Practical Course – I

Basic Practical Chemistry (Compulsory) **Practicals: 22 (Credits-4)**

Time allotted: Two practical sessions of 4 hours per week for one semester (one practical session for Section-I and one practical session for Section-II per week is compulsory)

SECTION-I: Physical Chemistry Practical (11 Experiments)

1. Statistical treatment of experimental data (calculation of mean and standard deviation for given data and least square method for calibration curve method) (compulsory)

Part-I: Chemical Kinetics: (Any three)

2. Kinetic decomposition of diacetone alcohol by dilatometry.
3. Determination of an order of a reaction.
4. Brönsted primary salt effect.
5. Kinetics of oxidation of ethanol by $K_2Cr_2O_7$

Part-II: Non-Instrumental: (Any Three)

6. Determination of surface excess of amyl alcohol or TX-100 surfactant by Capillary rise method.
7. Determination of molecular weight by steam distillation.
8. Glycerol radius by viscosity.
9. Partial Molar Volume (Polynometry) Determination of the densities of a series of solutions and to calculate the molar volumes of the components.

Part-III: Colorimetry and spectrophotometry (Any four experiments)

10. Simultaneous determination of Ni and Co by spectrophotometry (Ref-1)
11. Simulations determination of KMnO4 and K2Cr2O7 by spectrophotometry.(Ref-7)
12. To study the adsorption of certain dyes such as methyl violet, picric acid or malachite green on charcoal. (Ref-2)
13. To determine the indicator constant of bromocresolpuple by half height method (Ref-8)
14. Estimation of Cu(II) by titration with Na2 EDTA by colorimetry
15. a. Determination of energy of n to Π* transition in acetone and study of effect of solvent on energy of this transition by recording absorbance spectra in n-hexane and water. b. To study the effect of the extended conjugation on the λmax of p-nitro phenol by recording spectrum in acidic and alkaline medium (Ref-8).

Part -IV: Radioactivity: (Any one)
10. Estimation of Mn in tea leaves by NAA.
11. Half-life of a radioactive nuclide and counting errors.
12. Determination of E-max of β radiation and absorption coefficients in Al.

References:

1. Practical physical chemistry, A. Findlay, T.A. Kitchner (Longmans, Green and Co.)
2. Experiments in Physical Chemistry, J.M. Wilson, K.J. Newcombe, A.r. Denko. R.M.W. Richett(Pergamon Press)
3. Senior Practical Physical Chemistry, B.D. Khosla and V.S. Garg (R. Chand and Co., Delhi.).
4. Experimental Physical Chemistry by D. P. Shoemaker, Mc. Growhill, 7th Edition, 2003.
5. Physical chemistry by Wien (2001)
6. Advance Physical Chemistry Experiment, Gurtu and Gurtu, Pragati Publication (Meerut),
7. Experiments in Chemistry, D. V. Jahagirdar, Himalaya Publishing House
8. Practical physical Chemistry, B. Vishwanathan and P. S. Raghwan, Viva Books

Section-II: Organic Chemistry (11 Experiments)

Part-I: Purification Techniques (Compulsory) (8 Experiments)
a) Purification of two organic solids by recrystallization using water and alcohol.
b) Purification of two organic liquids by upward/downward/traditional distillation technique
c) Purification of organic compounds by column chromatography
d) Isolation of Eugenol from clove using steam distillation
e) Thin Layer Chromatography technique (two mixtures)
f) Sublimation by Cold Thumb Method

Part-II: Introduction to Green Chemistry (Compulsory 1 Practical)
Green Chemistry Experiments (any two)
1. Preparation of Schiff's bases in aqueous medium.
2. Preparation of acetanilide from aniline and acetic acid using Zn dust
3. Adoption of green method for functional group conversion
4. Mechanochemical solvent free, solid–solid synthesis of azomethine using p- toluidine and o-vanillin/p-vanillin (various other combinations of primary amine and aldehyde can also be tried).
5. Drawing of different chemical structures using Chemdraw software.

Self-Learning
1. Introduction to Laboratory Safety: Meaning of safety signs on container of chemicals, safety handling of chemicals, MSDS sheets: Detailed explanation at least for 4 different types of substances (e.g. nitric acid, benzene, potassium dichromate, bromine, etc.), Handling of glassware's and care to be taken, handling of organic flammable as well as toxic solvents in laboratory, use of safety goggles, shoes and gloves, fire extinguisher and its use, action to be taken in accidental cases e.g. cleaning of acid spill over, use eye wash station and bath station in emergency, etc.

2. Concept of green chemistry, applications of green chemistry

Examination Scheme:

1. The examination structure will be given before the commencement of examination.
2. Use of only supplied procedure will be allowed at the time of examination.
3. One experiment from Physical chemistry and any one experiment from organic section will be assigned.

Semester-II

Course code and Title: PSCH-121, Physical Chemistry-II

(Molecular Spectroscopy and Nuclear Chemistry) Lectures: 60 (Credits-4)

SECTION – I (2 Credits, 30 Hours)

Molecular Spectroscopy

1) Microwave Spectroscopy (06 Hours)

Introduction, Broadening of spectra, spectral intensities, types of molecule on the basis of moment of inertia, derivation of moment of inertia, rotational spectra of di- and polyatomic molecules.

2) Infra-red Spectroscopy (06 Hours)

The vibrating diatomic molecule, harmonic and an-harmonic oscillator, The diatomic vibrating rotator, breakdown of the Born-Oppenheimer approximation, The vibrations of polyatomic molecule, Fourier transform spectroscopy and its advantages, The carbon dioxide laser, Applications.

3) Raman Spectroscopy (06 Hours)

Quantum and classical theory of Raman effect, pure rotational Raman spectra, vibrational Raman spectra, polarization of light and Raman effect, structure determination from Raman and Infra-red spectroscopy, applications.

4) Electronic Spectroscopy of molecules (06 Hours)

Electronic spectra of diatomic molecules - The Born- Oppenheimer approximation, Vibrational coarse structure, Frank- Condon principle, dissociation energy and dissociation product,

5) Mossbauer Spectroscopy (06 Hours)

Principle, Instrumentation and Applications of Mossbauer Spectroscopy.

SECTION – II (2 Credits, 30 Hours)

Nuclear and Radiation Chemistry

1) Radioactivity (06 Hours)

Types of radioactive decay, general characteristics of radioactive decay, decay kinetics, general expression for the activity of a daughter nuclide, Geiger- Nuttalis law, α-decay: A problem in classical physics, Internal conversion and the Auger effect.

2) Elements of Radiation (06 Hours)

Chemistry: Interaction of radiation with matter, interaction of γ radiation with matter, units for measuring radiation absorption, Radiation dosimetry, Radiolysis of water,

3) Nuclear Fission: (07 Hours)

The discovery of nuclear fission, the process of nuclear fission, fission fragments and their mass distribution, charge distribution, Ionic charge of fission fragments, fission energy, fission cross-section and threshold, fission neutrons, theory of nuclear fission, Neutron evaporation and spallation.

4) Applications of Radioactivity (09 Hours)

Typical reaction involved in the preparation of radioisotopes, The Szillard- Chalmers reaction, Radiochemical principles in the use of tracers, Isotopes in elucidating reaction mechanism and structure determination, physic-chemical research - The solubility of a sparingly soluble substances, surface area of a powder or precipitate rates of diffusion,

Analytical applications- Isotope dilution analysis, Neutron activation analysis, Radiometric titrations, Medical applications-Thyroiditis, Assessing the volume of blood in a patient, Industrial applications thickness measurements and control, friction and wear out, gamma Radiography, Agricultural applications- Use of radiocalcium (^{45}C) and radio phosphorous (^{32}P) for the study of uptake rate of minerals from soil.

5) Introduction to Nuclear Forensic Chemistry (02 Hours)

References:

1) Elements of Nuclear Chemistry by H. J. Arnikar
2) Source book of Atomic energy by S. Glasstone and D. Van
3) Chemical applications of radioisotopes by H.J.M. Brown
4) Fundamentals of molecular spectroscopy by C.N.Banwell and E M McCash
5) Chapter on Nuclear and Radiochemistry by Dr. P D Sonawane in the edited book Innovations in Chemistry to Mankind, SCIENG Publications, Wardha

Course code and Title: PSCH-122, Inorganic Chemistry-II

Coordination and Bioinorganic Chemistry Lectures: 60 (Credits-4)

SECTION-I (2 Credits, 30 Hours)

Coordination Chemistry

Learning outcomes:

1. Student should able to find out the no of microstates and meaningful term symbols, construction of microstate table for various configuration
2. Hund's rules for arranging the terms according to energy.
3. Student should understand interelectronic repulsion.
4. Student should know the concept of weak and strong ligand field.
5. Student able to find out splitting of the free ion terms in weak ligand field and

strong ligand field.
6. To draw correlations diagram for various configurations in Td an Oh ligand field.
7. Student should know basic instrumentation and selection rules and relaxation in rules.
8. Student should know basic d-d transition, d-p mixing, charge transfer spectra.
9. Interpretation of electronic spectra for spin allowed oh and td complexes using Orgel diagram.
10. Understand the concept of Spectro chemical series and Nephelauxetic series.
11. Should able to solve numerical based on crystal field parameters.
12. Understand the various terms involved in magnetochemistry.
13. Various phenomenon of magnetism and their temperature dependence.
14. Various experimental methods to find out magnetic moment.
15. Understand the various Quenching of orbital angular momentum.

1. Concept and Scope of Ligand Fields: (06 Hours)

Quantum numbers, Free ion Configuration, Terms and States, Energy levels of transition metal ions, free ion terms, microstates, term wave functions, spin-orbits coupling.

2. Ligand Field Theory of Coordination Complexes (08 Hours)

Effect of ligand field on energy levels of transition metal ions, weak cubic ligand field effect on Russell- Saunders terms, Orgel diagrams, strong field effect, correlation diagrams, Tanabe-Sugano Diagrams, Spin-Pairing energies.

3. Electronic spectra of Transition Metal Complexes (08 Hours)

Introduction, band intensities, band energies, band width and shapes, transition metalspectra of 1^{st}, $2^{nd}$and 3^{rd} row ions and complexes, electronic spectra of Lanthanide and Actinide, spectrochemical and nephelauxetic series, charge transfer and luminescence spectra, calculations of Dq, B, β parameters, percentage of covalent character for metal complexes.

4. Magnetic Properties of Coordination Complexes (08 Hours)

Origin magnetism, types of magnetism, Curie law, Curie-Weiss Law, Magnetic properties of complexes-Para magnetism,

$1^{st}$and 2^{nd} Ordered Zeeman effect ,quenching of orbital angular momentum by Ligand fields, Magnetic properties of A, E and T ground terms in complexes, spin freeand spin paired equilibria, temperature dependence of magnetism.

References:

1. Ligand field theory and its applications by B.N. Figgis and M.A. Hitachman
2. Symmetry and spectroscopy of moleculesby K. Veera Reddy
3. Elements of Magnetochemistry by R. L. Datta and A. Syamal

Section-II: (2Credits, 30 Hours)
Bioinorganic Chemistry

Learning outcomes:

1) Importance of bioinorganic chemistry.
2) Role of metals in Metalloprotein and metalloenzymes.
3) Similarities in coordination theory for metal complexes and metal ions complexed with biological ligands.
4) Importance and transport of metal ions.
5) Passive transport metal ions by ionophores and gramicidin.
6) Mechanism for active transport of Na^+ and K^+
7) Introduction to biological nanoparticles, and Inorganic and bioinorganic Nanoparticles with help of ferritin, hemaoglobin , ion –channels.

1. Overview of Bioinorganic Chemistry (05 Hours)

Historical Background and current relevance, role of Cu, Fe, Mn and Mo in metallo-protein, and metalloenzymes.

2. Concepts of Inorganic Chemistry in Bioinorganic Chemistry (09 Hours)

Thermodynamic aspects - HSAB concept, chelate effect and Irving-William series, pK_a values of coordinated ligands, Tuning of redox potential, Biopolymer effects. Kinetic aspects- Electron transfer reaction, Electronic substitution reaction. Reactions of coordinated ligands and Template effect, concept of spontaneous self-assembly model compounds.

3. Functions and Transport of Alkali and Alkaline Earth Metal Ions (06 Hours)

Importance of alkali and alkaline earth metals, Distribution of cationic and anionic electrolytes in blood plasma and intracellular fluid, Ionophores: Natural and Synthetic, Application of ionophores, Different mechanism involved in exchange of ions across cell wall, Na+/K+-ATPase ion pump for active transport of Na^+ and K^+.

4. Biological Inorganic nano-particles and it's applications (10 Hours)

Introduction to biological nanoparticles, Exosomes, lipoproteins, Ferritin, Biological nano-moters and machines: Biological nano-machines: muscle myosin, ATPase, Hemoglobin. Biological nanoparticles production - plants and microbial Biological nanometers: Bacterial Flagella,cilia: Structure and function. Biological Nano-pores:Ion channels:bactrio-rhodopsin.

b) Applications: semiconductor, solar cell, top down and bottom up approach,

References:

1. Principle of Bioinorganic Chemistry by S.J. Lippard and J. M. Berg Bioinorganic Chemistry: Inorganic Elements in Chemistry of Life by W.Kaim and B. Schwederski.
2. Nanomaterials: by Dr. Sulbha Kulkarni.

3. The chemistry of Nanomaterials: by C. N. R. Rao , A. Muller, A. K. Cheetham Wiely – VCH verlag GmbH& Co. Volumes 1 & 2 .
4. Nanomaterials: Inorganic and Bioinorganic Perspectives
5. Charles M. Lukehart (Editor), Robert A. Scott (Editor) ISBN: 978-0-470- 51644-7

Course code and Title: PSCH – 123, Organic Chemistry-II

Lectures: 60 (Credits-4)

SECTION-I (2 Credits, 30 Hours)

Photochemistry and Pericyclic Reactions

Learning outcomes:

1. Students should able to understand free radicals' formation, stability and reactivity and should also be able to use the basic understanding in writing probable reaction mechanisms.
2. Students should able to write MO diagram for various olefinic compounds and should able to predict the products, the stereochemistry as well as should able to understand the preferred reaction pathways.
3. Students should able to calculate λ_{max} of organic compounds containing more than one and less than four conjugated systems. Students should able to correlate IR bands with functional groups using numerical data as well as spectral data.
4. Students should able to solve ^{1}H-NMR problems and should also able to draw the ^{1}H-NMR

1) Photochemistry (15 Hours)

Principles of Photochemistry, photochemistry of carbonyl compounds, alkenes, dienes, and aromatic compounds, photo rearrangements, Barton reaction, Patrno Buchi [2+2] cycloaddition reaction, photo redox reactions

Self-Learning; Photochemistry of Vision

2) Pericyclic Reactions (15 hours)

Electrocyclisation, cycloaddition, sigmatropic rearrangements and other related concerted reactions. Analysis by correlation diagrams, FMO approach, ene reactions, 1,3-dipolar additions.

Self-Learning: Group transfer reactions.

References:

1. Advanced Organic Chemistry, Part A by F. A. Carey and R. J. Sundberg
2. Excited states in Organic Chemistry by J.A. Barltrop and J.D.Coyle
3. Organic photochemistry: A visual approach by Jan Kopecky
4. Conservation of orbital symmetry by R. B. Woodward and R. Hoffmann
5. Orbital Symmetry: A problem solving approach- R. E. Lehr and A. P. Marchand
6. Pericyclic Reactions By A. P. Marchand, Roland E. Lehr
7. Organic reactions and orbital symmetry, 2nd Ed. T. L. Gilchrist and R. C. Storr
8. Molecular Orbitals and Organic Chemical Reactions by Ian Fleming

9. Pericyclic Reactions by Ian Fleming
10. Pericyclic Reactions by A Mechanistic and Problem-Solving Approach by Sunil Kumar Vinod Kumar S.P. Singh
11. Essentials of Pericyclic and Photochemical Reactions by Dinda and Biswanath
12. Pericyclic Reactions - A Textbook: Reactions, Applications and Theory by S. Sankararaman, Roald Hoffmann (Foreword by)

SECTION-II (2 Credits, 30 Hours)
Spectroscopic Methods in Structure Determination of Organic Compounds

1. UV Spectroscopy (02 Hours)

UV: Recapitulation of UV spectroscopy, Calculations of λ_{max} of aromatic compounds.
Self learning: Calculations of λ_{max} of polyenes and α,β-enone.

2. IR Spectroscopy (04 hours)

Hooks law, types of vibrations, Near IR, Far IR, Finger print and functional group region, IR spectra of important functional groups 1. With and without conjugation, 2. Ring size effect 3. Effect of H-bonding, 4. Resonance effect 5. Inductive effect.

3. ^{1}H-NMR (14 Hours)

Basic principle of NMR, Chemical and Magnetic equivalence and nonequivalence, Homotopism, Enantiotopism, diastereotopism, chemical shifts and factors influencing chemical shift: electronegativity, NMR solvent polarity, temperature, anisotropic effect, chemical shifts of acidic protons, D_2O exchange, Multiplicity patterns and Coupling Constants: Pascal's triangle, tree diagram, complex splitting patterns in aromatic, vinylic, and saturated monocyclic compounds, Introduction to NMR of racemic mixture, relationship between integration and ee% in diasterotomers.
Problems: complex problems based on multiple coupling constants should be discussed and drawing of expected ^{1}H-NMR spectrum along with complex multiplicity and coupling constants.

4. ^{13}C-NMR (04 Hours)

Basic of 13C-NMR: Chemical shift and factors affecting chemical shifts in 13C NMR, off resoanance and proton noise decoupled spectra. Simple problems on ^{13}C-NMR.

5. Mass spectrometry (MS) (06 Hours)

Basic principle of MS, significance of M^+ (m/z) in determination of molecular formula, Rule of 13, Nitrogen Rule, Base peak and Molecular ion peak, isotopic abundance. Genesis of m/z fragments: alkanes (cyclic and acyclic), alcohols, amines.
Problems: Based on 2-3 fragments of above mentioned functional groups should be discussed.
Combined problems: Problems based on UV, IR, MS, ^{1}H-NMR, ^{13}C-NMR should be solved.
Self-Learning: Genesis of simple molecules

References:

1. Introduction to Spectroscopy by Donald L. Pavia and Gary M. Lampman
2. UV-VIS Spectroscopy and Its Applications by Perkampus, Heinz-Helmut
3. Infrared Spectroscopy: Fundamentals and Applications by Barbara H. Stuart
4. Infrared Spectroscopy by James M. Thompson
5. Spectrometric Identification of Organic Compounds by Robert M. Silverstein, Francis X. Webster, David J. Kiemle, David L. Bryce
6. Introduction to Spectroscopy by Donald L. Pavia
7. Understanding NMR Spectroscopy by James Keeler
8. Spin Dynamics: Basics of Nuclear Magnetic Resonance by Malcolm H. Levitt
9. Guide to Spectroscopic Identification of Organic Compounds by Karen Feinstein
10. Principles of Nuclear Magnetic Resonance in One and Two Dimensions by Richard R. Ernst, Geoffrey Bodenhausen, Alexander Wokaun
11. NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry by Harald Günther
12. Basic One- and Two-Dimensional NMR Spectroscopy by Horst Friebolin
13. Principles of Nuclear Magnetism by A. Abragam
14. Principles of Magnetic Resonance by Charles P. Slichter
15. Nuclear Magnetic Resonance by Peter Hore
16. Applications of NMR Spectroscopy by Atta-ur-Rahman, M. Iqbal Choudhar
17. Solving Problems with NMR Spectroscopy by Atta-ur-Rahman Muhammad Choudhary Atia-tul- Wahab

Course code and Title: PSCHELE – 124, General Chemistry -II

Lectures: 60 (Credits-4)

SECTION-I: Theory Course (2 Credits, 30 Hours)

(Any one option is to be selected by candidate)

Elective Option-A: Material Characterization Technique

Learning outcomes:

At the end of course student will understand / able to explain

1. Different characterization technique of solids.
2. Principle of XRD, instrumentation of powder XRD, Brags law, applications of XRD for crystal structure determination, numerical problems.
3, Principle of XRF, types of XRF, instrumentation, qualitative and quantitative analysis,
4. Principle of SEM, instrumentation of SEM and interpretation of surface morphology of solid from SEM.
5. Principle of TEM, instrumentation of TEM and interpretation of TEM images.
6. Principle and instrumentation of scanning probe microscopy

7. Principle of thermal analysis, types of thermal analysis, instrumentation, qualitative and quantitative analysis.

1. X-Ray Diffraction Methods (12 Hours)

Miller and Weiss indices, Features of Characteristic X-Rays, Types of Characteristic X-Rays, Selection Rules, Comparison of K, L, and M Series, Generation of X-Rays, X-Ray Absorption, Theoretical Background of Diffraction, Diffraction Geometry, Bragg's Law, Reciprocal Lattice, Diffraction Intensity, Structure Extinction, X-Ray Diffractometry, Instrumentation, System Aberrations, Samples and Data Acquisition, Sample Preparation, Acquisition and Treatment of Diffraction Data, Distortions of Diffraction Spectra, Crystallite Size, Applications, Crystal-Phase Identification, Quantitative Measurement , Wide-Angle X-Ray Diffraction and Scattering, Wide-Angle Diffraction, Wide-Angle Scattering. Problem on XRD (Calculation of d values, assigning planes, calculation of crystal parameters)

Features of Characteristic X-Rays, Types of Characteristic X-Rays, Selection Rules, Comparison of K, L, and M Series, X-Ray Fluorescence Spectrometry, Wavelength Dispersive Spectroscopy, Analyzing Crystal, Wavelength Dispersive Spectra, Energy Dispersive Spectroscopy, Detector, Energy Dispersive Spectra.

2. Transmission Electron Microscopy (04 Hours)

Instrumentation, Electron Sources, Thermionic Emission Gun, Field Emission Gun, Electromagnetic Lenses , Specimen Stage, Specimen Preparation, Prethinning, Final Thinning, Electrolytic Thinning, Ultramicrotomy, Image Modes (Mass–Density Contrast, Diffraction Contrast, Phase Contrast), Selected-Area Diffraction (SAD), Selected-Area Diffraction Characteristics.

3. Scanning Electron Microscopy (04 Hours)

Instrumentation, Optical Arrangement, Signal Detection, Detector, Probe Size and Current Contrast Formation, Electron–Specimen Interactions, Topographic Contrast, Compositional Contrast, Operational Variables, Working Distance and Aperture Size, Acceleration Voltage and Probe Current, Astigmatism, Specimen Preparation, Preparation for Topographic examination.

4. **Scanning Probe Microscopy (06 Hours)**

Instrumentation, probe and scanner, control and vibration isolation, Scanning tunnelling microscopy and atomic force microscopy

4. Thermal Analysis (04 hours)

Common characteristic, Thermal events, instrumentation, experimental parameters, DTA and DSC, working principles, Measurement of temperature and enthalpy changes, Applications, Thermogravimetry, Instrumentation, applications

References:

1. Yang Leng, Materials Characterization -Introduction to Microscopic and Spectroscopic Methods, Second Ed. Wiley-VCH,

2. R. D. Braun, Introduction to Instrumental Analysis, Second Ed.

3. Elaine A. Moore, Lesley E. Smart - Solid State Chemistry - an Introduction. Fourth Ed. CRC Press (2012)

Elective Option - B: Organometallic and Inorganic Reaction Mechanism

Learning Outcomes:

At the end of course students will able to explain

1. Valence electron count, back bonding in organometallics, spectral characterization of organometallic compounds.
2. Catalytic reaction involving organometallic compounds and mechanism of these reactions
3. Types of reaction involving organometallic compounds
4. Types of reactions in coordination compounds, inert and labile complexes, substitution reactions in coordination complexes and their mechanism, stereochemistry of reaction, kinetics of reactions.

1. Organometallic Chemistry **(10 Hours)**

Organic ligands and nomenclature, 18 electron rule: counting electrons, ligands having extended pi system, bonding between Metal Atoms and organic pi systems: linear pi system, cyclic pi system, **s**pectral analysis and characterization of organometallic complexes: IR and NMR, examples.

2. Organometallic Reactions and Catalysis **(10 Hours)**

Reactions involving gain and loss of ligands: ligand dissociation and substitution, oxidative addition, reductive elimination, nucleophelic displacement, **r**eactions involving modification of ligands: insertion, carbonyl insertion, 1-2 insertion, hydride elimination, abstraction, organometallic catalysis: Hydroformylation, Monsanto acetic acid process, Wacker Process, Hydrognation by Willkinsons catalyst, Olefin metathesis, heterogeneous catalysis: Ziegler Natta Polymerization, Water gas reduction.

3. Coordination Compounds: Reactions and Mechanism **(10 hours)**

History and principles, Substitution reactions: Inert and labile complexes, mechanism of substitution, Kinetics Consequences of reaction pathway: dissociation, interchange, association, Experimental evidences in Octahedral Substitution: dissociation, linear free energy relationship, associative mechanism, the conjugate base mechanism, the kinetic chelate effect, Stereochemistry of reactions: substitution in trans complexes, substitution in cis complexes, isomerisation of chelate rings, substitution reactions in Sq. Pl. Complexes.

Reference

1) Inorganic Chemistry: Gary Miessler and Donald A. Tarr, Third Ed., Pearson (Chapter-12, 13 and14 pages: 422 to 561)

2) IUPAC Nomenclture of Organometallic Compounds of Transition Metals by Salzer http://publications.iupac.org/pac/1999/71_08_pdf/7108salzer_1557.pdf

Elective Option– C: Introduction to Chemical Biology-II

Learning outcomes:
The goal of this course is to introduce students to fundamental concepts in Chemical Biology and methods of chemistry used to solve problems in molecular and cell biology. After completion of this course, successful students will:
1) Students will be able to explore new areas of research in both chemistry and allied fields of science and technology.
2) Students will be able to function as a member of an interdisciplinary problem solving team.
3) To impart the students thorough idea in the chemistry of carbohydrates, amino acids, proteins and nucleic acids etc.
4) Be able to describe the chemical basis for replication, transcription, translation and how each of these central processes can be expanded to include new chemical matter.
5) Develop skills to critically read the literature and effectively communicate research in a peer setting.
6) Describe the importance of chemical biology research and interdisciplinary work.

1. Enzymes **(08 Hours)**
Classification w.r.t. reaction catalysis, Theory of Enzyme -Substrate (ES) formation, Active sites and its features, Enzyme specificity, Factors affecting enzyme activity, enzyme Kinetics (MM equation, LBW equation), Allosteric enzymes, Types of enzyme inhibition, Industrial applications of enzymes

2. Nucleic Acid **(08 Hours)**
Central dogma of molecular biology, Differences between DNA and RNA, Overview of replication transcription, Genetic code, translation, Gene cloning, Gene Therapy, Applications of Biotechnology

3. Metabolism of Biomolecules **(08 Hours)**
Aerobic and Anaerobic glycolysis, TCA Cycle, Beta oxidation of fatty acids, Trans amination, deamination, decarboxylation of amino acids, Urea cycle

4. Biochemical Techniques **(06 Hours)**

Protein purification and characterization, Dialysis, Chromatography, Electrophoresis, Native and SDS-PAGE

References:
1. Principals of biochemistry, Albert Lehninger (CBS Publisher and Distributers Pvt. Delhi.
2. Harper's Biochemistry by R.K. Murray, D. I. Granner, P. A. Mayes, (Prentice Hall International Inc.)
3. Biochemistry by U. Satynarayana
4. Biochemistry by J. L. Jain
5. Biophysical Techniques by Upadhyaya Nath

Course code and Title: PSCHPELE-124

SECTION-II: Practical Course **Practicals: 11 (Credits-2)**

(Any one option to be selected by candidate)

Elective Option-A: Electrochemical Methods of Analysis

Time allotted: One practical Session of 4 hours per week for one semester

Total 11 practical to be conducted

Part-I: Conductometry: (Any three)

1. Hydrolysis of NH4Cl or CH3COONa or aniline hydrochloride.
2. Determination of λ0 or λα and dissociation constant of acetic acid.
3. Hydrolysis of ethyl acetate by NaOH.
4. Determination of ΔG, ΔH, and ΔS of silver benzoate by conductometry.
5. Determination of critical micellar concentration (CMC) and ΔG of micellization of sodium Lauryl Sulphate / Detergent

Part-II: Polarography (any one)

6. Determination of half wave potential E 1/2 and unknown concentration of Cu or Pb or Zn ion.
7. Amperometric titration of Pb(NO3)2 with K2Cr2O7.

Part-III: Potentiomerty: (Any three)

8. Stability Constant of a complex ion.
9. Solubility of a sparingly soluble salt.
10. To determine the ionic product of H2O
11. Estimation of halide in mixture.

Part-IV: pH metry (any two)

12. Determination of the acid and base dissociation constant of an amino acid and hence the isoelectric point of the acid.
13. Determination of dissociation constants of tribasic acid (phospheric acid)
14. Construct pH curve for titration of strong base – strong acid, strong base - weak acid and predict the best indicator in these titrations (methyl orange, methyl orange, brocresol green, phenolphthalein, etc.)

Part-V: Table Work (any two)

15. Analysis of powder XRD of SrTiO3 and Ag metal or any two compounds (Calculation d, lattice constant, crystal volume and density, and assigning planes to peaks using JCPDS data)
16. Cyclic voltamogram of K3Fe(CN)6 in KCl/H2O / Ferrocene in TEAP//MeCN
17. Detailed interpretation of Raman spectra of diatomic molecules

References:

1. Practical physical chemistry, A. Findlay, T.A. Kitchner (Longmans, Green and Co.)
2. Experiments in Physical Chemistry, J.M. Wilson, K.J. Newcombe, A.r. Denko. R.M.W. Richett(Pergamon Press)
3. Senior Practical Physical Chemistry, B.D. Khosla and V.S. Garg (R. Chand and Co., Delhi.).
4. Experimental Physical Chemistry by D. P. Shoemaker, Mc. Growhill, 7th Edition, 2003.
5. Physical chemistry by Wien (2001)
6. Advance Physical Chemistry Experiment, Gurtu and Gurtu, Pragati Publication (Meerut)
7. Experiments in Chemistry, D. V. Jahagirdar, Himalaya Publishing House
8. Practical physical Chemistry, B. Vishwanathan and P. S. Raghwan, Viva Books

Examination Scheme:
1. The examination structure will be given before the commencement of examination.
2. Use of only supplied procedure will be allowed at the time of examination.

Elective Option-B: Chemical Biology-II Practical
Time allotted: One practical Session of 4 hours per week for one semester

Perform at least 11 Practical
1. Dialysis and Reverse dialysis of protein salt solution
2. Separation of protein by Gel filtration method
3. Separation of protein by affinity chromatography method
4. Separation of protein by Ion exchange chromatography
5. Native and SDS PAGE of proteins
6. Separation of amino acids by paper chromatography
7. Separation of nucleic acid by Agarose gel electrophoresis
8. Effect of pH on enzyme activity
9. Effect of Temperature on enzyme activity
10. Effect of substrate concentration on enzyme activity
11. Detection of λ Max of proteins
12. Detection of λ Max of Nucleic acid

References:
1. A reference book of Biochemistry Practicals by Sadashivam
2. Practical approach to biochemistry by Plummer
3. Martin Holtzhauer, Basic Methods for the Biochemical Lab, First Edition, Springer

Course Code and Title: PSCHP-125: Practical Course-II

Basic Practical Chemistry (Compulsory) **Practicals: 22 (Credits-4)**

Time allotted: Two practical sessions of 4 hours per week for one semester (one practical session for Section-I and one practical session for Section-II per week is compulsory)

Section-I: Inorganic Chemistry (11 Experiments)

Part-I: Synthesis of coordination complexes (any three) (Ref. 2)
1. Synthesis and Purity of [Mn(acac)3]
2. Synthesis and Purity Chloropentaamminecobalt(III) chloride.
3. Synthesis and Purity Nitro pentaamminecobalt(III) chloride.
4. Synthesis of Phthiocol (2-hydroxy-3-methyl-1,4-napthaquinone) and their complex with Zn or Cd and Purity of the complex.

Part-II: Inorganic Conductometry (any two)
4. Structural determination of metal complexes by conductometric measurement. (Ref-3)
5. To study complex formation between Fe(III) with sulfosalicylic acid by conductometry (Ref-3).
6. To verify the Debye Huckel theory of ionic conductance for strong electrolytes KCl, BaCl2, K2SO4 and [K3Fe(CN)6] (Ref-3)
7. Determination of Pb(II) in solution with Na2SO4 solution and determination of solubility product of PbSO4 (Ref-4)

Part-III: Inorganic characterization techniques (any two of the following)
8. Determination of equilibrium constant of M – L systems Fe(III)–Sulphosalicylic acid or Fe(III)–β–resorcilic acid by Job's continuous variation method. (Ref.-3, 5)
9. Solution state preparation of [Ni(en)3]S2O3, [Ni(H2O)6]Cl2, [Ni(NH3)6]Cl2. Record absorption spectra in solution of all three complexes and calculate 10 Dq. Arrange three ligands according to their increasing strength depending on your observations. (Ref. -5)
10. Determination of magnetic susceptibility (χg and χm) of mercury tetracyanato cobalt or Fe(acac)3 or Ferrous ammonium sulfate by Faraday or Gouy method. (Ref. -3, 5)

Part-IV: Inorganic Kinetics Experiment (any two)
11. Synthesis and photochemistry of K3[Fe(C2O4)3].3H2O. (Ref-4)
12. Kinetics of substitution reaction of [Fe(Phen)3]2+ (Ref-3)
13. Kinetics of formation of Cr(III)-EDTA complex (Ref-3)

Part-V: Ion – Exchange Chromatography (Ref. -1 and 3)
1. Separation of mixture of Zn(II) and Mg(II) using Amberlite IRA 400 anion exchanger and quantitative estimation of separated ions Zn(II) and Mg(II)

Part-VI: Solvent Extraction and colorimetric (any one experiment) (Ref. -1 and 3)
2. Determination of Cu(II) by solvent extraction as Dithiocarbamate complex (Ref-1)
3. Determination of iron by solvent extraction techniques in a mixture of Fe(III) +Al(III) or Fe(III) + Ni(III) using 8–hydroxyquinoline reagent. (Ref. -1)

References:
1. Vogel's Textbook of Inorganic quantitative analysis
2. Experimental Inorganic Chemistry, Mounir A. Malati, Horwood Series in Chemical Science (Horwood publishing, Chichester) 1999.

3. Students are made aware of carrying out different types of reactions and their workup methods.

4. This practical course is designed to make student aware of green chemistry and role of green chemistry in pollution reduction

Examination Scheme:
1. The examination structure will be given before the commencement of examination.
2. Use of only supplied procedure will be allowed at the time of examination.
3. Any one experiment from inorganic chemistry and any one experiment from organic section will be assigned time the time of examination.

Section -II: Organic Chemistry (11 Experiments)

Learning Outcomes:
1. This course is designed to make students aware of how to perform organic compounds in laboratory.
2. The course includes synthesis of some derivatives and organic compounds, which will help them while working in research laboratory in future.
3. Making derivatives of organic compounds will help them in industry or while doing research in medicinal chemistry for Drug development.
4. This practical course is also designed to make student aware of green chemistry and role of green chemistry in pollution reduction.
5. The students learn how to avoid solvents and do solvent free reaction.
6. Also the work-up procedure in many experiments is made more eco-friendly to environment.

1. Bromination of trans-stilbene using sodium bromide and sodium bromate
2. [4+2] cycloaddition reaction in aqueous medium at room temperature
3. Benzil Benzilic acid rearrangement under solvent free condition
4. Ultrasound-assisted synthesis of 7-hydroxy-4-methylcoumarin
5. Eco-friendly nitration of phenols and its derivatives using Calcium nitrate
6. Bromination of acetanilide using ceric ammonium nitrate in aqueous medium
7. Green approach for preparation of benzopinacolone from bezopinacol using iodine catalyst
8. Preparation of 1, 1-bis-2-naphthol under grinding at room temperature.
9. Solvent free aldol condensation between 3,4-dimethoxybenzaldehyde and 1- indanone
10. Isolation of Trimyristin from nutmeg
11. Isolation of caffeine from tea leaves
12. Microwave-assisted reactions in water: Hofmann Elimination, methyl benzoate to benzoic acid and Decarboxylation reaction
13. Green Synthesis of the following compounds: adipic acid, catechol, disodium iminodiacetate (alternative to Strecker synthesis)

Note: Students should perform a) Relevant chemical analysis. b) Column chromatography. c) Elemental analysis. d) Spectroscopic interpretation. e) How to draw schemes and mechanism using Chem Draw / ISIS Draw etc.

N B. :
1. Use molar concentrations for volumetric /estimations/synthesis experiments.

2. Use optimum concentrations and volumes
3. Two burette method should be used for volumetric analysis (Homogeneous mixtures)
4. Use of microscale technique is recommended wherever possible

References:

1. Comprehensive Practical Organic Chemistry by V.K. Ahluwalia and Renu Aggarwal
2. Monograph on Green Chemistry Laboratory Experiments by Green Chemistry TaskForce Committee, DST

Course Outcomes:

1. Students are trained to different purification techniques in organic chemistry like recrystallization, distillation, steam distillation and extraction.
2. Students are made aware of safety techniques and handling of chemicals.
3. Students are made aware of carrying out different types of reactions and their workup methods.
4. This practical course is designed to make student aware of green chemistry and role of green chemistry in pollution reduction.

Examination Scheme:

1. The examination structure will be given before the commencement of examination.
2. Use of only university supplied procedure will be allowed at the time of examination.
3. Any one experiment from inorganic chemistry and any one experiment from organic section will be assigned time the time of examination.

Pattern of Question Paper

For theory courses, end semester question papers will be set by the College and centralized assessment for theory papers done as per the rules laid down by the College. Questions will be designed to test the conceptual knowledge and understanding of the basic and advanced concepts of the subject. There will be **two sections** for each paper. Each section will be of **35 marks** and the pattern of question paper shall be:

Question 1 (10 Marks)	5 compulsory sub-questions, each of 2 marks; precisely answerable in 2-5 sentences (such as define, short problem, draw the structure / neat labelled diagram, short reasons, characteristics, applications, etc.)
Question 2 (10 Marks)	2 out of 4 – descriptive answer type questions of 5 marks each; answerable in sufficient length with graph or diagram or flow sheet if necessary.
Question 3 (10 marks)	2 out of 4 – Critical analysis / differentiation / evaluative / summarize interpret, write notes, numerical problem type of questions of 5 marks each; answerable in 15 lines with graph or diagram if applicable.
Question 4 (5 Marks)	1 out of 2 – numerical problem type question; spectral analysis, For descriptive course critical notes, decryption of technique, how you will apply your knowledge to solve particular problem, etc. types of question.

In question paper setting wattage for each chapter will be proportional to number of theory lectures assigned to that chapter.