Savitribai Phule Pune University

(Formerly University of Pune)

Post-Graduate Program in Chemistry

(Faculty of Science and Technology)

New Syllabi (As Per National Education Policy-2020) of

M.Sc. (Chemistry) Part-I

(Organic Chemistry and Drug Chemistry)

(For Colleges Affiliated to Savitribai Phule Pune University)

To be implemented with effect from Academic Year 2023-2024

1. Preamble:

The global education development agenda reflected in the Goal 4 (SDG4) of the 2030 Agenda for Sustainable Development, adopted by India in 2015 - seeks to "ensure inclusive and equitable quality education and promote lifelong learning opportunities for all". Such a towering goal will require the entire education system to be redesign to support and foster learning, so that all of the critical targets for Sustainable Development can be achieved. National Education Policy 2020 is the first education policy of the 21st century and aims to address the many growing developmental imperatives of our country. This Policy proposes the revision and revamping of all aspects of the education structure, including its regulation and governance, to create a new system that is aligned with the aspirational goals of 21st century education, including SDG4. The NEP 2020 is based on the principle that education must develop critical thinking and problem solving abilities along with social, ethical, and emotional capacities.

The M.Sc. Chemistry syllabi is revised as per the guidelines of UGC, Government of Maharashtra and Savitribai Phule Pune University, Pune. With NEP-2020 in background, the revised curricula will articulate the spirit of the policy by emphasizing upon- integrated approach to learning; innovative pedagogies and assessment strategies; multidisciplinary and Interdisciplinary education; creative and critical thinking; student-centric participatory learning; imaginative abilities and flexible curricular structures to enable creative combination of disciplines for the study. The M.Sc. Chemistry Programme will transmit advanced knowledge of chemical sciences along with its fundamentals. In this programme, students will be empowered with assignments in academia and industry to provide the skills and information necessary for creating employment. The Programme exposes students to significant advances in chemical sciences as well as related fields through multidisciplinary and interdisciplinary courses. The design of the syllabi is such a way that it addresses chemical safety, green chemistry principles and industrial skills. It is intended to bring out the best in each student's ability, to sharpen their scientific temper, and to keep them up to date on recent developments in the field.

The Aims of the programme are:

a) To impart basic and advanced knowledge of chemical sciences among students.
b) To provide adequate blend of theory, computation and hands-on experiments.
c) To provide higher education, disciplinary and inter/multi-disciplinary research oriented knowledge to the students.

d) To provide a learned, skilled and creative pool of graduates who are ready to take up challenging assignments in different kinds of chemical industries, research institutions and academia.

e) To foster responsible, proactive individuals who are equipped with rational thinking and competencies to address local challenges.

The M.Sc. Chemistry course structure consists of a well-balanced mix of Major Core, Major Electives, Research oriented courses, On-Job training/Internship and Project based learning. Out of total of 88 credits, 18 credits have been allotted to Research methodology and Project based learning. For M.Sc. Chemistry Degree, a student has to earn the minimum 88 credits from their four semesters. If students complete 44 credits in PG first year, he/she can exit with PG Diploma or continue with PG second year. The M.Sc. Chemistry course structure is based on following credit framework as per the guidelines of the university and government of Maharashtra.

Credit Framework for M.Sc. Chemistry Programme

Level	**Semester**	**Credits Related to Major**		**Research Methodology (RM)**	**Internship Job Training (OJT)**	**Research Project (RP)**	**Total**
6.0	I	10 (T) + 4 (P)	2 (T) + 2 (T/P)	4	0	0	**22**
	II	10 (T) + 4 (P)	2 (T) + 2 (T/P)	0	4	0	**22**
Exit Option: Award of PG Diploma on Completion of 44 credits at 6.0 level (PG First Year) or Continue with PG Second Year							
6.5	III	10 (T) + 4 (P)	2 (T) + 2 (T/P)	0	0	4	**22**
	IV	8 (T) + 4 (P)	2 (T) + 2 (T/P)	0	0	6	**22**
Total 4 Years		**54**	**16**	**4**	**4**	**10**	**88**
Abbreviation: T – Theory, P - Practical							

Guidelines for conduction of classes:

a) A student has to attend 1-hour classroom teaching per week for one credit of theory and 2 hours' lab work/problem-solving session/ related activities per week for one credit of practical. Practical sessions (lab work/problem-solving session/related activity) will be conducted in batches. A batch for such sessions will be of size maximum of 08 students.

b) 4 Credit courses will have 60 lectures (48 L + 12 T) and 2 Credit courses will have 30 lectures (24 L + 6 T)

c) The Department may conduct necessary lectures/workshops as a part of OJT.

d) Each course of 4 credits will carry 100 marks and 2 credit courses will carry 50 marks.

e) There will be Continuous Internal Evaluation (CIE) and Semester End Examination (SEE) for each course.

Evaluation process:

a) The CIE will be based on minimum two internal tests (IT). In addition, a teacher may consider one or more of the following. (i) Home Assignments (ii) Seminar/Presentation (iii) Laboratory assignment (iv) Group Discussions (v) Oral (vi) Research Paper/Book Review (vi) Technology Demonstration (vi) Case study (vii) Survey report, etc.

b) Students has to score a minimum of 40 % separately in CIE and SEE, otherwise the result of such a course will be FAIL.

Eligibility:

B.Sc. Chemistry/B.Sc. (Blended) Chemistry/ B.E./B.Tech. with Chemistry subject (at least in second year) as per the rules and regulations given by Savitribai Phule Pune University, Pune.

2. Programme Outcomes (POs)

PO No.	PO Statement After completing the Master of Science degree students are able to	Knowledge and Skill
PO-1	Learn the terms, theories, assumptions, methods, principles, theorem statements and classification	Disciplinary knowledge
PO-2	Fix out the problem and resolve it using theories and practical knowledge.	Critical thinking and Problem solving
PO-3	Inculcate knowledge for carrying projects and advanced research related skills.	Research related skill
PO-4	Actively participate in team on case studies and field-based situations.	Cooperation/Team work
PO-5	Analyze and interpret ideas, evidences and experiences with learned scientific reasoning	Scientific reasoning
PO-6	Aware and implement the subject facts that can be applied for the personal and social development	Reflective thinking
PO-7	Use digital literacy to retrieve and evaluate subject related information	Information/Digitally literacy
PO-8	Get moral and ethical values for society as well as in research	Moral and ethical awareness
PO-9	Give analytical reasoning to interpret research data.	Analytical Reasoning
PO-10	Improve their managerial skills and abilities in subject related activities.	Leadership readiness/qualities
PO-11	Inculcate continuous learning habit through all available resources.	Lifelong readiness/qualities

3. Programme Specific Outcomes (PSOs)

PO-No.	Outcomes	Component
PSO-1	Demonstrate a comprehensive knowledge of all disciplines.	Disciplinary knowledge
PSO-2	To assess and evaluate facts, claims and arguments using their scientific knowledge	Critical thinking
PSO-3	To define a problem, analyse, interpret and draw conclusion by planning, implementing and reporting the results of an experiment.	Research-related skills
PSO-4	To access, evaluate and apply a variety of useful sources	Information/digital literacy
PSO-5	To participate in multicultural society and communicate the subject knowledge for the betterment of society	Multicultural competence
PSO-6	To acquire knowledge and skills including "Learning how to learn" that are necessary in learning activities throughout life	Lifelong learning

4. Course Structure

M. Sc. Chemistry Part-I

(Organic Chemistry and Drug Chemistry)

Semester I

Sr. No.	Course Title	Course Code	Major Core/ Major elective	Credits
1	Physical Chemistry-I	CHE-501	Major Core	4
2	Inorganic Chemistry-I	CHEOD-502	Major Core	2
3	Organic Chemistry-I	CHE-503	Major Core	4
4	Physical Chemistry Practical -I	CHE-504	Major Core	2
5	Inorganic Chemistry Practical-I	CHE-505	Major Core	2
6	Organic Chemistry Practical-I	CHE-506	Major elective	2
7	Chemical Mathematics	CHE-507(A)	Major elective	2
	Chemistry of Nanomaterials	CHE-507(B)		
	Analytical Chemistry	CHE-507(C)		
	Organic Reactions and Reagents	CHEOD-507(D)		
8	Research Methodology	CHE-508	RM	4

Semester II

Sr. No.	Course Title	Course Code	Major Core/ Major elective	Credits
1	Physical Chemistry-II	CHEOD-551	Major Core	2
2	Inorganic Chemistry-II	CHE-552	Major Core	4
3	Organic Chemistry-II	CHE-553	Major Core	4
4	Physical Chemistry Practical -II	CHE-554	Major Core	2
5	Inorganic Chemistry Practical-II	CHE-555	Major Core	2
6	Organic Chemistry Practical-II	CHE-556	Major elective	2
7	Organometallic Compounds and Inorganic Reaction Mechanism	CHE-557(A)	Major elective	2
	Material Characterization Techniques	CHE-557(B)		
	Green Chemistry	CHE-557(C)		
	Nuclear and Radiation Chemistry	CHEOD-557(D)		
8	On-Job Training/Internship	CHE-558	OJT/Internship	4

5. Detailed Syllabus

Semester I

CHE- 501, Physical Chemistry I (4 Credits, 60 L)

Section I [2 Credits, 30 L T]

Chapter 1: Thermodynamics (15 L)

State function, path function, exact and inexact differential, Maxwell's relationship, temperature and pressure dependence of thermodynamic quantities, Clausius inequality, chemical potential, variation of chemical potential with temperature and pressure, chemical potential in a system of ideal gases, Determination of partial molar quantities, Methods for the determination of molar quantities, Thermodynamics of mixing, Entropy of mixing, Numerical problems

Chapter 2: Quantum chemistry (15 L)

Recapitulation, Schrodinger wave equation, particle in one dimensional box, particle in three dimensional box, Degeneracy, Normalization and orthogonality of wave functions, one dimensional simple harmonic oscillator, operators- Algebra of operators, commutator operator, linear operators, operator ∇ and ∇^2, hydrogen like atom (no deviation), Numerical problems

Section II [2 Credits, 30 L]

Chapter 1: Chemical kinetics (20 L)

Rate law: Recapitulation, the temp dependent reaction rate, reaction moving towards equilibrium, consecutive reactions, parallel reactions, pre equilibria, unimolecular reactions. Numerical problems.

Kinetics of complex reactions: The steady state approximation, chain reactions, free radical polymerization, reaction between H_2 and Br_2, explosive reactions, Numerical problems.

Molecular reaction dynamics: Collision theory of bimolecular, gas phase reactions, diffusion controlled and activation-controlled reaction in solution, activated complex theory of reaction rate, Eyring equation. Numerical problems.

Enzyme catalysis: Introduction, Michaelis Menten mechanism, effect of pH and temperature on enzyme catalysed reactions, limiting rate, Lineweaver -Burk, Eadie-Hofstee methods and plots, competitive and non-competitive inhibition, Numerical problems.

Chapter 2: Molecular Thermodynamics (10 L)

Molecular energy levels, Boltzmann distribution law, partition functions and ensembles, translational, rotational and vibrational partition function of diatomic molecules, Thermodynamic properties in terms of partition functions (internal energy, heat capacity, entropy and equilibrium constant), Maxwell-Boltzmann, Fermi- Dirac and Bose -Einstein statistics.

References:

1. Physical chemistry by Peter Atkins, Julio De Paula, 11th Edition , 2018, Oxford University Press
2. Principals of Physical chemistry by Puri Sharma Pathania, 48th edition, Vishal Publishing Co.
3. Physical chemistry by GM borrow, 5th edition , 2006, Mc Graw Hill Education
4. Quantum chemistry by Ira Levine, 6th Edition
5. Quantum chemistry by R.K. Prasad, 4th Edition
6. Physical chemistry by biological sciences by Raymond Chang (Page Number 113, 135, 141)
7. Principles of Physical Chemistry by Marron and Prouton, 4th edition
8. Physical Chemistry: A Molecular Approach by by Donald A. McQuarrie, John D. Simon (20 August 1997)

Course Outcomes

CO1: Students should be able to remember the concepts of thermodynamic parameters, quantum mechanical postulates, rate laws of chemical reactions and computation of macroscopic properties of matter.

CO2: Students should understand the basics like state function and path function, Schrodinger wave equation, kinetics of fast reactions, partition functions and ensembles.

CO3: Students should be able to apply the knowledge of various quantum mechanical methods to determine the different molecular properties and built the concept of the relation between thermodynamics and quantum mechanics.

CO4: Students should be able to analyze the rates of various chemical reactions both theoretically and experimentally and also observe the effect of catalyst and determine energies of activation of such reactions.

CO5: Students should be able to evaluate variation of thermodynamic parameters for multi component systems and their variation with other extensive properties, Schrodinger wave equation and its application to hydrogen and hydrogen like atoms.

CO6: Students should be able to create the solutions to avoid excess use of energy in chemical reactions by applying their knowledge of thermodynamics and chemical kinetics.

CHEOD-502, Inorganic Chemistry-I (2 credits, 30 L)

(Molecular Symmetry and its applications to Inorganic chemistry)

Chapter-1: Molecular Symmetry and Symmetry Groups (12 L)

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

Chapter-2. Representations of Groups (08L)

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

Chapter-3: Symmetry Adapted Linear Combinations (05L)

Projection operators and their use of construct SALC (Construction of SALC for sigma bonding for molecules belonging point groups D2h, D3h, D4h, C4v, Td, Oh normalization of SALC, transformation properties of atomic orbital, MO's for sigma bonding, ABn molecules, tetrahedral AB4 and Oh AB6 cases.

Chapter-4: Application of Group theory to Infrared Spectroscopy (05L)

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

References:

1. Chemical Applications of Group Theory by F. A. Cotton Third Edition, (Wiley, New York)
2. Symmetry and Spectroscopy of Molecules by K. Veera Reddy Second Edition 2009: (New Age International Publication)
3. Group Theory and its Chemical Application, P.K. Bhattacharya
4. Symmetry in Chemistry by H. Jaffe and M. Orchin, Himalaya Pub.House-New Delhi,

Course Outcomes: At the end of course student should able to -

CO-1: Define symmetry elements and symmetry operations, classes, properties of a group,group multiplication table, etc.

CO-2: Classify symmetry elements, point group, Group, sub-group and classes.

CO-3: Use wave function as basis for determination of irreducible representations and the GreatOrthogonality theorem and its consequence.

CO-4: Solve problem based on point group, matrix representation and character table

CO-5: Construct character table of various point group

CO-6: Justify which can take part in bonding on the basis of SALCs and point group of molecules.

CHE-503, Organic Chemistry-I (4 credits, 60 L)

(Organic Reaction Mechanism, Stereochemistry and Reagents)

Section-I (2 credits, 30 L)

Chapter-1: Nature of Bonding in Organic Molecules (12 L)

a) Structure and Bonding:

1. Recapitulation: Various structural and electronic effects, strength of acids and bases and pKa and pKb

2. Electron Donor–Acceptor (EDA) complexes, crown ether complexes and cryptates, catenanes and rotaxanes, inclusion compounds, fullerenes

Ref. 1

b) Aromaticity:

1. Recapitulation: Benzenoid and non-benzenoid compounds, aromaticityand Huckel's rule

2. Antiaromaticity Quasiaroamtic and homoaromatic compounds, application to carbocyclic and heterocyclic systems, annulenes, azulenes and fulvenes, mesoionic compounds, current concepts of aromaticity, Frost Musulin Diagram

Ref. 1 and 2

Problem solving

c) Reactive Intermediates:

1. Recapitulation: Intermediate and transition state, carbocations, carbanions, benzyne, free radicals

2. Generation, structure, stability and reactivity of carbenes, nitrenes, ketene and isocyanate

Ref. 1, 2 and 3

Problem solving

Chapter-2: Stereochemistry (18 L)

1. Recapitulation: Origin of stereochemistry, optical activity, chirality. Projection formulae, Conformational concepts, conformations of acyclic & cyclic (ethane, propane, butane, cyclohexane, methylcyclohexane) molecules.
2. Stereoisomerism, enantiomeric relationship, distereomeric relationship, % ee and % de, D/L, R/S and E/Z nomenclature in C, N, S, P containing compounds, prochiral relationship, Re/Si faces, Topicity, optical activity in biphenyls, spiranes, allenes, helical structures, ansa compounds and cyclophanes, stereospecific and stereoselective reactions, stability and optical activity in cis and trans decalins, stereochemical aspects of elimination (E2 and Ei) and addition reactions (syn and anti-additions).

Ref. 4, 5 and 6

Problem solving

Section-II (2 credits, 30 L)

Chapter 1: Aliphatic Nucleophilic Substitution reactions (8 L)

1. S_N1, S_N2 and S_Ni reactions (Mechanism, Reactivity and Stereochemical aspects)

Ref. 1

2. Neighbouring group participation: The neighbouring group mechanism, The Neighbouring group participation by π and σ bonds, NGP by halogens and heteroatoms (O, N, S), anchimeric assistance, classical and non-classical carbocations, phenonium ions, norbornyl system, carbocation rearrangements in neighbouring group participation.

Ref. 7 and 8

Problem solving

Chapter 2: Aromatic electrophilic and nucleophilic substitution reactions (10 L)

1. Recapitulation: Mechanism of aromatic electrophilic substitution reaction.
2. Orientation effects in aromatic electrophilic substitution reactions (Benzene, Naphthalene, Anthracene, Pyridine, Pyrrole, Furan and Thiophene)
3. Kolbe, Gatterman, Gatterman-Koch, Riemer-Tieman, Vilsemeyer-Haack, Hoesch, Ipso substitution.
4. Benzyne reaction, Meisenheimer complex, cine and tele substitutions, Chichibabin reaction, Sandmeyer Reaction

Ref. 1, 2, 3 and 8

Problem solving

Chapter 3: Oxidation and Reduction Reactions (12 L)

1. Recapitulation: CrO_3 (Jones reagent), $KMnO_4$, O_3, OsO_4, $LiAlH_4$, $LiBH_4$, $NaBH_4$,
2. Oxidising reagents: PDC, PCC, MnO_2, Swern, $Pb(OAc)_4$, RuO_4, Woodward and Prevost dihydroxylation, peracid, HIO_4, TEMPO, IBX, CAN, Fetizon's Reagent
3. Reducing reagents: $NaBH_4/CeCl_3$, $NaBH_3CN$, Willkinsons catalyst, DIBAL, Clemenson, Wolff-Kishner reduction, Rosenmund Reduction, Birch, dissolving metal, Lindlar catalyst

Ref. 8, 9, 10, 11

Problem solving

References

Essential books

1. Advanced Organic Chemistry, Reactions Mechanisms and Structure by J. March, 6th edition, John Wiley

2. Advanced Organic Chemistry Part A: Structure and Mechanism and Part B: Reaction and synthesis, Francis A. Carey, Richard J. Sundberg, 5th Edition, Springer
3. Advanced organic chemistry, Jagdamba Singh and LDS Yadav, 1st Edition, Pragati Prakashan.
4. Stereochemistry of Organic Compounds (Principles and Applications) by D. Nashipuri, 4th edition, New Age International Private Limited.
5. Stereochemistry of Organic Compounds by by Ernest L. Eliel and Samuel H. Wilen, 1st edition, Wiley.
6. Stereochemistry: Conformation and Mechanism by P.S. Kalsi, 11th Edition, New Age International Private Limited.
7. Mechanism and Structure in Organic Chemistry by E.S. Gould, 1st Edition, Holt, nehart and Winston of Canada Ltd.
8. Organic Chemistry, Jonathan Clayden, Nick Geeves, Stuart Warren, 1st Edition, Oxford University Press
9. Modern Synthetic Reactions by Herbert O. House, 1st Edition.
10. Advanced Organic Chemistry Part B: Reactions and Synthesis by Francis A. Carey and Richard J. Sundberg, 5th Edition, Springer.
11. Organic Synthesis by Jagdamba Singh, L.D.S Yadav, Pragati Prakashan.

Further reading

1. A Guidebook to Mechanism in Organic Chemistry by Peter Sykes, 6th Edition, Pearson Education.
2. Reaction Mechanism in Organic Chemistry by S. M. Mukherji, 3rd edition, Laxmi Publications.
3. Organic Reactions and Their Mechanisms by P.S. Kalsi, 5th edition, New Age International Private Limited.
4. Principles of Organic Synthesis by R.O.C. Norman and J.M. Coxon, 3rd Edition.

Course Outcome: Student will able to –

CO1: Understand the concepts of chemical bonding, various structural effects, acids and bases, intermediates and aromaticity.

CO2: Learn the concepts of stereochemistry.

CO3: Understand and identify the types of organic reactions.

CO4: Advanced knowledge of various stereochemical aspects.

CO5: Establish mechanistic knowledge of aliphatic and aromatic substitutions, and oxidation-reduction reactions

CO6: Develop problem solving ability of the students.

CHE- 504, Physical Chemistry Practical I [2 Credits, 60 L]

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.To investigate the rate constant of an autocatalytic reaction between potassium permanganate and oxalic acid.

Part-II: Non-Instrumental (Any three)

6. Partial Molar Volume (Polynometry) Determination of the densities of a series of solutions and to calculate the molar volumes of the components.

7.Determination of molecular weight by steam distillation.

8. To determine the radius of Glycerol molecule by viscometry.

9.Isotherm for a three-component system: chloroform/acetic acid /water.

Part-III: Colorimetry and Spectrophotometry (Any four)

10.Spectrophotometric determination of the acid dissociation constant of methyl red

11.Simultaneous determination of $KMnO_4$ and $K_2Cr_2O_7$ by spectrophotometry.

12.To study the adsorption of certain dyes such as methyl violet, picric acid or malachite green on charcoal.

13.To determine the indicator constant of bromocresol puple by half height method 14. 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

Part -IV: Radioactivity

15.Determination of E-max of β radiation and absorption coefficients in Al.

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. 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.).

Course outcomes:

CO1: Students will grasp the concept of reaction rate and its significance in Chemical Kinetics.

CO2: Students will learn how to use experimental data to deduce rate laws and rate constants.

CO3: Students will be familiar with the fundamental principles of colorimetry and spectrophotometry including Beer's law, Lambert- Beer's law and the relationship between absorbance and concentration.

CO4: Students will be able to operate the instruments like spectrophotometer and colorimeter.

CO5: Students will be able to determine the densities of the solutions and can calculate molar volumes

CHE-505, Inorganic Chemistry Practical-I (2-Credits; 60 L)

(Inorganic Material analysis, Synthesis and Its Applications)

Part-1: Ore Analysis (Any two) (Ref.1)

1. Determination of silica and manganese from pyrolusite ore.
2. Determination of aluminium and silica from bauxite ore.
3. Determination of silica and iron from hematite ore
4. Determination of copper and sulphide from chalcopyrite ore.

Part-2: Alloy Analysis (Any two) (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 cupra-nickel alloy
8. Determination of copper and zinc from brass alloy.

Part-3: Synthesis of materials/ nanomaterials and their applications (Any six)

9. Synthesis of ZnO from zinc oxalate precursor method and determine band gap by absorption spectroscopy (Ref. 2-4, 6).
10. Heterogeneous Photo-Catalysis: Removal and kinetics of photo-catalytic dye degradation (methylene blue) on synthesized ZnO. (Ref. 5)
11. Synthesis of TiO_2 by Sol-Gel method and determine band gap by absorption spectroscopy (Ref-4)
12. Heterogeneous Photo-Catalysis: Removal and kinetics of photo-catalytic dye degradation (methylene blue) on synthesized TiO_2. (Ref. 5)
13. Synthesis of colloidal silver nanoparticles (suspension) and determine band gap by absorption spectroscopy. (Ref. 3-4)
14. Synthesis of Cu_2O nanoparticles of different colours. (Ref. 7)
15. Synthesis of MnO_2 (Ref. 2)
16. Heterogeneous Catalysis: Study on decomposition of H_2O_2 by non -catalysed and MnO_2 catalysed method (Ref. 2, 12)
17. Synthesis of CuxS nano-particles. (Ref. 9-11)
18. Study of non-stoichiometry of synthesised CuxS (Estimation of Cu(II) by colorimetry)
19. Synthesis of Fe_2O_3 nanoparticles from FeC_2O_4. (Ref. 2 and 8)
20. Heterogeneous Catalysis: Study on decomposition of H_2O_2 by non-catalysed and Fe_2O_3

catalysed method (Ref. 2, 8 and 12).

Part-4: Table Work (compulsory)

1. Study of MnO_2 / Fe_2O_3 / ZnO / TiO_2 / Silver – nanoparticles or any other materials:
2. Powder XRD analysis with respect to - 2θ from XRD, miller indices to assigned using JCPDS or ICDD data and experimentally observed 2θ, inter planar distance, crystal volume,lattice parameters.
3. **SEM:** Write surface morphology and calculate grain size.

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. Text book of Quantitative Analysis, A.I. Vogel 4th Edn. (1964).
2. Experimental Inorganic Chemistry, Mounir A. Malati, HorwoodSeries in Chemical Science(Harwood publishing, Chichester) 1999
3. A Laboratory Course in Nanoscience and Nanotechnology; Dr. Gérrard Eddy Jai Poinern;CRC Press Taylor & Francis, 2015
4. Nanotechnology: Principles and Practices, Sulbha Kulkarni, Springer, (2015)
5. Environmental Chemistry Microscale laboratory Experiments, Jorge G. Ibanez Margarita Hemandez-Esparza, Carmen Doria-Serrano, Arturo Fregoso-Infante, Mono Mohan Singh, Springer, 2008.
6. Ecofriendly synthesis and solar photocatalytic activity of S-doped ZnO; Journal of Hazardous Material, Volume 183, Issues 1–3, 15 November 2010, Pages 315-32310.1016/j.jhazmat.2010.07.026
7. Synthesis of Copper(I) Oxide Particles with Variable Color: Demonstrating Size-Dependent Optical Properties for High School Students; J. Chem. Educ; DOI: 10.1021/acs.jchemed.5b00563
8. Catalytic Efficiency of Iron(III) Oxides in Decomposition of Hydrogen Peroxide: Competition between the Surface Area and Crystallinity of Nanoparticles Martin Hermanek, Radek Zboril, Ivo Medrik, Jiri Pechousek, and Cenek Gregor, J. AM. CHEM. SOC. 2007,

129, 10929-10936,

9. CuS Nanoparticles Trigger Sulfite for Fast Degradation of Organic Dyes under Dark Conditions; *CS Omega* 2022, 7, 5, 4140-4149; **DOI:** 10.1021/acsomega.1c05697.
10. A facile chemical route to copper sulfide CuS nano-crystallites – pH effect of the morphology and the shape of them; journal of optoelectronics and advanced materials; Vol. 8, No. 2, April 2006, p. 597 – 60
11. Facial Grinding Method for Synthesis of High-Purity CuS Nanosheets; *Ind. Eng. Chem. Res.* 2018, 57, 8, 2759–2764; https://doi.org/10.1021/acs.iecr.7b04616
12. Practical Physical Chemistry, B. Vishwanathan and P. S. Raghwan, Viva Books (2005)

Course Outcomes: Student will able to -

CO-1: Prepare solution of required conc. and the handle laboratory equipment properly.

CO-2: Perform experiment accurately and able to perform calculation.

CO-3: Explain experiment and principal of experiment in detail.

CO-4: Perform calculations and discuss results and write conclusions of the experiment.

CO-5: Apply knowledge to a) design experiment for given aim or modify experiment to enhance results. b) to find out lacuna in experimental procedure.

CO-6: Solve problem/ numerical depending on given experimental data / information.

CHE-506, Organic Chemistry Practical I (2-Credits; 60 L)

(Single stage preparation and purification techniques)

Single stage preparation and Recrystallization (Any Seven)

1 Reduction of aromatic aldehyde using sodium borohydride.
(**Recrystallization**)

2 Vilsmeier-Haack reaction of N, N-dimethyl aniline.
(**Recrystallization)**

3 Bromination of acetanilide using Ceric Ammonium Nitrate
(**Recrystallization**)

4 Synthesis of dihydropyrimidinone using Biginelli reaction
(**Recrystallization**)

5 To study the Base catalyzed Aldol condensation using $LiOH.H_2O$ as catalyst
(**Recrystallization)**

7 Synthesis of p-chlorotoulene from p-toluidine by using Sandmeyer reaction.
(**Recrystallization**)

8 Synthesis of β-naphthyl methyl ether from β-naphthol.
(**Chemical Separation and Recrystallization**)

9 Reduction of p-nitrotoluene using Sn/HCl.
(**Chemical Separation and Crystallization**)

Single stage preparation and Simple Distillation (Any Two)

1 Purification of crude aniline by distillation and its conversion to acetanilide
(**Simple Distillation**)

2 Reduction of acetophenone using hydrazine hydrate.
(**Simple Distillation**)

3 In situ preparation of sodium hypochlorite (NaOCl) using bleaching powder and NaOH and its application in the oxidation of cyclohexanol to cyclohexanone.
(**Simple Distillation**)

Single stage preparation and Other Purification Techniques (Any Three)

1 Synthesis of phthalimide from phthalic acid.
(**Sublimation technique)**

2 Nitration of Phenol and Purification by Column Chromatography.
(**Column Chromatography**)

3 Cannizzaro reaction of substituted aromatic aldehyde.
(**Chemical Separation**)

4 Preparation of Aryloxy derivative of phenolic compound.
(**Separation by solvent extraction)**

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. Vogel's Textbook of Practical Organic Chemistry, 5th edition Pearson India.
2. Comprehensive Practical Organic Chemistry by V.K. Ahluwalia and Renu Aggarwal
3. Advanced Practical Organic Chemistry by John Leonard, John Leonard, Barry Lygo, Garry Procter, 2nd edition, CRC Press.
4. Solvent-free Organic Synthesis by Koichi Tanaka.
5. Practical Organic Chemistry by Mann and Saunders, 4th edition, Pearson Education.
6. Advanced Practical Organic Chemistry by John Leonard, Barry Lygo, Garry Procter, 3rd Edition.

Course Outcome: Student will able to -

CO1: Understand the theoretical aspects behind separation, purification and synthesis of organic compounds.

CO2: Acquire the experimental skills for separation, purification, identification and synthesis of organic compounds.

CO3: Design experimental set up for performing the organic reactions.

CO4: Monitor the organic reactions.

CO5: Describe the mechanistic aspects of organic reactions.

CO6: Develop problem solving ability.

Chemistry electives

(Any one option from the following four courses)

CHE – 507(A), Chemical Mathematics (2 credits, 30)

Chapter 1: Functions (**14 L**)

Differential and integral calculus, limits, derivatives, physical significance, basic rules of differentiations, maxima and minima, exact and inexact differentials, partial differentiations, rules of integrations, substitution, applications to chemistry related problems.

Chapter 2: Differential Equations **(08 L)**

Separation of variables, homogeneous, exact, linear equations of second order, series solution method.

Chapter 3: Vectors, Matrices and Determinants **(08 L)**

Vectors, dots, cross and triple products, Introduction to matrix, algebra, addition and multiplication of matrices, inverse adjoints and transport of Matrices, unit and diagonal matrices.

References

1) Chemical maths book, E. Steiner

2) Maths for chemistry vol 1,2 Martin M C R Cockette and G.Doggett.

3) Mathematical preparations for physical chemistry F. Daniels, Mc Graw Hill.

4) Principles of Physical chemistry by Puri Sharma Pathania

Course Outcomes: After studying the chemical mathematics, the students can learn

CO1: Students will able to remember rules of differentiation, integration, vectors, matrices and determinants.

CO2: Students can understand the various rules to solve problems related to derivatives, integration, vectors, matrices and determinants.

CO3: Students able to apply mathematical concepts to solve problems related to chemistry.

CO4: Students can analyse the chemical problems using the knowledge of integration, differentiation, vectors, matrices and determinants.

CO5: Students can evaluate various chemical problems can evaluate by using rules of integration, differentiation, vectors, matrices and determinants.

CO6: Students will able to create chemical problems with methods of mathematical background

CHE-507(B), Chemistry of Nanomaterials(2 Credits) (30 L)

Chapter-1: The Big World of Nanomaterials (03 L)

History and Scope; Can Small Things Make a Big Difference? Classification of Nanostructured Materials; Fascinating Nanostructures; Applications of Nanomaterials; Nature: The Best Nanotechnologist; Challenges and Future Prospects (Ref. 1: 1 to 25)

Chapter-2: Band Theory (04 L)

Metallic Bonding and Band Theory; Band structure of metals; Band structure of insulators; Band structure of semiconductors: silicon; Band structure of inorganic solids, III–V, II–VI and

I–VII compounds, Transition metal compounds, Fullerenes and graphite, Bands or Bonds: a Final Comment

Ref-1-66-100; Ref.-2: 173-186

Chapter-3: Defects in Nano-structure and Properties of Nanomaterials (06 L)

Types of Defect: perfect and imperfect defects, Point Defects, Schottky defect, Frenkel defect, The Kroger–Vink notation for crystal defects, Colour centres, Vacancies and interstitials in non-stoichiometric crystals: extrinsic and intrinsic defects, Defect clusters or aggregates, Interchanged atoms: order–disorder phenomena Extended Defects, Crystallographic shear structures, Stacking faults, Sub-grain boundaries and antiphase domains (boundaries).

Ref. 1: 29 to 36; Ref. 2: 83 to 86; 90-95; 108 to 116; 120 to 123;

Chapter-4: Effect of Nano-Dimensions on Materials Behavior (06 L)

Elastic properties; Melting point; Diffusivity; Grain growth characteristics, Enhanced solid solubility, Magnetic properties, Soft magnetic nanocrystalline alloys, Giant magnetoresistance (GMR), Electrical properties, Mechanical properties, Hardness and strength, Tensile ductility and strain hardening, Creep and superplastic behaviour, Fracture and toughness, Corrosion properties. Ref. 1: 36 to 66). Ref-5: 1-29

Chapter-5: Synthetic Methods of Nanomaterials (06 L)

General Observations; Bottom up and top-down approach (definitions); Solid State Reaction or Shake ’n Bake Methods: Nucleation and growth, epitaxy and topotaxy, Practical considerations and some examples of solid state reactions, Combustion synthesis, Mechano-synthesis; Low Temperature or Chimie Douce Methods: Alkoxide sol–gel method (Synthesis of $MgAl_2O_4$, Synthesis of silica glass, Spinning of alumina fibres, Preparation of indium tin

oxide (ITO) and other coatings), Preparation of indium tin oxide (ITO) and other coatings, Sol–gel method using oxyhydroxides and colloid chemistry (Synthesis of zeolites, Preparation of alumina-based abrasives and films, Citrate gel and Pechini processes, Use of homogeneous, single-source precursors, Hydrothermal and solvo-thermal synthesis, Microwave synthesis, Intercalation and deinter-calation, Graphite intercalation compounds, Pillared clays and layered double hydroxides, Example of a difficult synthesis made possible by chimie douce methods: $BiFeO_3$.

Ref-1: 66-106; Ref. 2: 187 to 225.

Chapter-6: Applications of Nanomaterials (05 L)

1. Photocatalysis: Material name, working and principle of Photocatalysis, 2. Gas sensing - Material name, working and principle of gas sensor, 3. Medical applications, 4. coloured nanomaterials as inorganic pigments, 5. Nano catalysis- Material, its application and mechanism 6. Nanomaterials of environmental pollution remediation. 7: Fuel Cell, 8. Photovoltaic Cell.

Ref. 1. 108 to 148; Ref. 5: 29 to 43, Ref. 6

References

1. Textbook of Nanoscience and Nanotechnology, B S Murty P Shankar Baldev Raj B B Rath James Murday, Springe/University press, 2013.
2. Solid State Chemistry and its Applications, Anthony R. West, Second Edition Student Edition; Wiley, 2014
3. Chemistry of Nanomaterials Fundamentals and Applications, Tahir Iqbal Awan, Almas Bashir, Aqsa Tehseen, Elsevier, 2020.
4. Solution Methods for Metal Oxide Nanostructures, Rajaram S Mane, Vijaykumar V Jadhav, Abdullah M Al-Enizi; Elsevier, 2023.
5. Advanced Nanomaterials and Their Applications in Renewable Energy Jingbo Louise Liu, Sajid Bashir; Elsevier (2015).
6. Research Papers: a) Photocatalysis: From Fundamental Principles to Materials and Applications; *ACS Applied Energy Materials* 2018 *1* (12), 6657-6693; DOI: 10.1021/acsaem.8b01345 b) Photocatalysis for Organic Wastewater Treatment: From the Basis to Current Challenges for Society; Catalysts 2020, 10, 1260; doi:10.3390/catal10111260; c) Gas sensing mechanism of metal oxides: The role of ambient atmosphere, type of semiconductor and gases - A review, Sci. Lett. J. 2015, 4: 126, d) Review: Influences of Semiconductor Metal Oxide Properties on Gas Sensing

Characteristics; https://doi.org/10.3389/fsens.2021.657931 e) An Overview of Nanomaterials for Water and Wastewater Treatment; Advances in Materials Science and Engineering Volume 2016, Article ID 4964828, 10 pages http://dx.doi.org/10.1155/2016/4964828

Course Outcomes: At the end of course student will able to-

CO-1. Define / memories the terms related to - applications of nanomaterials, band theory, defects in crystal structures, some properties of nanomaterials, synthesis of nanomaterials.

CO-2. Discuss Applications of nanomaterials, synthesis methods of nanomaterials, some properties of nanomaterials, defects in nanomaterials.

CO-3. Apply their knowledge to – choose synthesis method for nanomaterial, selection of nanomaterial for particular application, explain observed properties of nanomaterial, etc.

CO-4. Differentiate / compare – metals-semiconductors-insulators, Non-stoichiometry and point defects, different synthetic methods, properties of nanomaterials.

CO-5. Explain the terms related to - applications of nanomaterials, band theory, defects in crystal structures, some properties of nanomaterials, synthesis of nanomaterials.

CO-6. Propose scope / Applications of nanomaterials to solve real problems.

CHE-507(C), Analytical Chemistry (2 credits, 30 L)

Chapter 1: Good Laboratory Practice: Quality Assurance of Analytical Measurements (10 L)

Good Laboratory Practice, Validation of Analytical Methods, Quality Assurance, Laboratory Accreditation, Electronic Records and Electronic Signatures: 21 CFR, Part 11, Official Organization.

Chapter 2: Lab Safety (08 L)

Laboratory Emergencies: Spills and Fires I. General Preparation for Emergencies- Handling the Accidental Release of Hazardous Materials, Notifications, Spill Containment and Clean-up, Leaking Gas Cylinders, Fires, Classification, Fire Extinguishers (how they work, types), Risk Assessment, Case Study, Sources of chemical hazards, hazards of organic synthesis, sulphonating hazard, organic solvent hazard. Control measures for chemical hazards. Management of combustible gases, toxic gases and oxygen displacing gases, Regulations for chemical hazards, MSDS, labelling guidelines, management of overexposure to chemicals and TLV concept, and Disposal of hazardous material.

Chapter 3: Mass Spectrometry (12 L)

Principle, instrumentation, ionization methods- electron bombardment ionization, arc and spark ionization, Photo-ionization, thermal ionization, Chemical ionization, Mass analyzers- Magnetic, double focusing, Time of flight, Quadrupolar, Ion cyclotron resonance analyzer, Correlation of mass spectra with molecular structure and molecular weight, Isotopic Abundances, Fragmentation patterns, Quantitative analysis, Applications and Problems. Fourier transform mass spectrometry, Tandem mass spectrometry, inductively coupled Plasma-mass spectrometry, Secondary ion–mass spectrometry and ion microprobe mass analyzer.

References

1. Introduction to Instrumental Analysis, R. D. Braun, Mc Graw-Hill. Inc.1987.
2. Instrumental Methods of Chemical analysis, H. H. Willard, L. L. Merritt Jr., J. A. Dean and F. A. Settle Jr., 6th Edition, Wadsworth Publishing Company, USA,1986
3. Fundamentals of Analytical Chemistry, D. A. Skoog, D. M. West, F. J. Holler, S. R. Crouch, 7th Edition, Thomson Asia Pte. Ltd, Singapore,2004
4. Instrumental Methods of Chemical Analysis – B. K. Sharma 26th Ed. 2007, pages 286-307

5. Good laboratory practice, regulations, 2nd Edition, Sandy, Wenberg, Vol.69, Marcel, Dekker series, 1995.
6. Daniel A. Crowl, Joseph F. Louvar, Chemical Process Safety; Fundamentals with application, 3rd edition, prentice hall, 2011.
7. Quantitative risk assessment in chemical process industries, American institute of chemical industries, centre for chemical process safety.

Course Outcome: Student will able to –

CO1: Define/memorize GLP, Lab Safety, Quality assurance

CO2: Discuss good laboratory practices, laboratory emergencies, and mass spectrometry

CO3: Apply their knowledge to prepare quality assurance reports, emergencies in the laboratory

CO4: Differentiate between different ionization technique, compare hazardous and non-hazardous material handling

CO5: Explain the Quality Assurance, Laboratory Accreditation, Laboratory Emergencies, different ionization technique

CO6: Applications of GLP, Lab Safety, mass spectrometry

CHEOD-507(D) Organic Reactions and Reagents [2 Credits, 30 L]

Chapter 1: Organic Reactions (15 L)

Acyloin condensation, Benzoin Condensation, Bamford-Stevens Reaction, Bergman Cyclisation, Chichibabin Reaction, Eschenmoser-Tanabe Fragmentation, Grob Fragmentation, Mitsunobu Reaction, McMurry Coupling, Nazarov cyclisation, Nef reaction, Robinson annulation, Shapiro Reaction, Stork enamine reaction

Problem solving

Ref. 1 to 5

Chapter 2: Reagents (15 L)

Grignard Reagent, Organo Zinc, Organo Copper and Organo lithium reagents, Ylides-Phosphorus, Nitrogen and Sulphur ylide

Problem solving

Ref. 6 to 8

References

1. Strategic Applications of Named Reactions in Organic Synthesis 1st Edition - Laszlo Kurti, Barbara Czako
2. Name Reactions-A Collection of Detailed Mechanisms and Synthetic Applications-Jie Jack Li
3. Name Reactions and Reagents in Organic Synthesis-by Bradford P. Mundy, Michael G. Ellerd, Frank G. Favaloro Jr.
4. Organic Syntheses Based on Name Reactions A Practical Encyclopedic Guide to Over 800 Transformations -4th Edition - Alfred Hassner, Irishi Namboothiri, Meir Golan
5. Name Reactions in Organic Synthesis by Arun Parikh
6. Organic Chemistry, Jonathan Clayden, Nick Geeves, Stuart Warren, 1st Edition, Oxford University Press
7. Organic Synthesis by Jagdamba Singh, L.D.S Yadav, Pragati Prakashan.
8. Advanced Organic Chemistry Part B: Reactions and Synthesis by Francis A. Carey and Richard J. Sundberg, 5th Edition, Springer.

Course outcomes: At the end of the course, students will be able to-

CO1: Understand the concepts of named organic reactions and reagents.

CO2: Identify the type of named organic reaction and uses of reagents.

CO3: Predict the reaction conditions of organic reaction.

CO4: Write the reaction mechanism.

CO5: Design appropriate synthetic route.

CO6: Develop problem solving ability of the students.

CHE-508, Research methodology (4 credits, 60 L)

Chapter-1: Introduction to Research methodology (02 L)

Objective of research, motivation in research, types of research, Fundamental research, applied research, experimental research, and interdisciplinary research.

Chapter-2: Scope of Research and Ethics (05 L)

Steps in scientific research: scientific methods of research, criteria of good research, and characteristics of a good research, Research problem: Identification, Selection, developing research title, Criteria for prioritizing topics for research, Prioritizing Topics for Research, Formulation of research objectives. Types and importance of research ethics, Institutional ethics committee, Plagiarism, Patenting and intellectual property rights. Publication ethics: definition, introduction, and importance.

Chapter-3: Literature Survey and Search technique (08L)

Print: Sources of information: Primary, secondary, tertiary sources; Journals: Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, and Formula Index.Literature Search technique**:** SCOPUS, Google Scholar, PUBMED, Web of Science, science direct, Indian Citation Index, Research Gate, and scifinder, Scirus, ChemIndustry, Wiki- Databases, ChemSpider.

Chapter-4: Overview of the journal article (06 L)

Selection of journals, Data bases and research metrics Databases: i) indexing databases

ii) Citation databases: Web of Science, Scopus, UGC-Care List etc.

Research Metrics: a) Impact Factor of journal as per Journal Citation Report, SNIP, SJR,IPP, Cite Score b) Metrics: h-index, g index, i10 index.

Chapter-5: Presentation of Scientific findings, Scientific Report Writing (09 L)

Publication Process: Types of technical documents- Full length research paper, Short/Brief communications, Letters to editor, Book chapter, Review, Conference report, Patents, dissertation. Components of a research publication: Title/Topic statement, Abstract/key words, Aims and objectives, Hypothesis building, Rationale of the paper, Work plan, Materials and methodology, Results and discussion, Key issues, and arguments, Acknowledgement, Conflict of interest statement, bibliography, Technical Resumes & Cover Letters. Softwares in Chemistry Data Plotting Structure Drawing, Grammar Checkers and Sentence Correction Tools.

Chapter-6: Data Analysis and interpretation (15 L)

The Investigative Approach: Making and Recording Measurements. SI Units and their uses, Scientific method and design of experiments, Analysis and Presentation of Data: Descriptive statistics. Choosing and using statistical tests. Chemometrics. Analysis of variance (ANOVA), Correlation and regression, Curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, General polynomial fitting, linearizing transformations, exponential function fit, r and its abuse, basic aspects of the multiple linear regression analysis.

Chapter-7: Presentation and Communication skills (05 L)

Tables, Figures and Pictures using Excel, PowerPoint slide preparation, Preparation of Posters, Electronic submission of manuscripts, oral and poster, Communication skills.

Chapter-8: Ethical Handling of Chemicals (10 L)

Safe working procedure and protective environment, protective apparel, emergencyprocedure and first aid, laboratory ventilation. Handling of various chemicals, solvents & glassware. Fires and fighting with fires. Hazardous substances, Safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards classification, and handling Safety Data Sheet. Chemical entries, MSDS, CAS numbers, dead stocks maintenance. Disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals.

References

1. C. R. Kothari, Research Methodology: Methods and Techniques, New Age International, 1990
2. B. L. Garg, R. Karadia, F. Agarwal and U. K. Agarwal, An introduction to Research Methodology, RBSA Publishers, 2002
3. S. M. Coley and C. A. Scheinberg, Proposal Writing, Sage Publications, 1990.
4. Research Methodology by Best and Kahn, PHI Limited.
5. Research Methodology by R. Kumar, A Step-By-Step Guide for Beginners,Pearson Education, Delhi (2006).
6. Fundamentals of modern statistical methods by Rand R.wilcox.
7. Power Analysis for Experimental Research A Practical Guide for the Biological,Medical and social Sciences by R. Barker Bausell, Yi-Fang Li Cambridge University Press.
8. Design of Experience: Statistical Principles of Research Design and Analysis,by Robert O. Kuehl Brooks/cole.
9. Panneerselvam R., Research Methodology, Prentice Hall Of India, New Delhi,2004

10. Design & Analysis of Experiments by D. C. Montgomery, 5th Ed., Wiley India (2007).

Course outcomes:

CO1: Develop a comprehensive understanding of different research methodologies and their applications in mathematics.

CO2: Cultivate critical thinking and analytical skills necessary for identifying research problems and formulating research questions.

CO3: Provide practical experience in designing experiments, collecting and analyzing data, and interpreting research results.

CO4: Foster effective communication skills for presenting research findings orally and in written form.

CO5: Promote ethical research practices and awareness of responsible conduct in mathematical research

CO5; Develop problem solving ability.

Semester II

CHEOD- 551, Molecular Spectroscopy (2 Credits, 30 L)

Chapter 1: Microwave Spectroscopy (06 L)

Rotation of molecules, Rotational spectra of diatomic molecules- rigid diatomic molecule, intensities of spectral lines, effect of isotopic substitution, non-rigid rotator, spectrum of non-rigid rotator, polyatomic molecules, linear molecules, symmetric top molecules, Asymmetric top molecules, Applications. Ref. 1 Pages 33-58

Chapter 2: Infra-Red Spectroscopy (06 L)

Vibrating diatomic molecule, diatomic vibrating rotator, vibration rotation spectrum of carbon monoxide, Breakdown of the Born-Oppenheimer approximation, vibration of polyatomic molecules, Fourier transform spectroscopy (FTIR) and its advantages, carbon dioxide laser and its advantages. Ref. 1 Pages 60-81, 102-110.

Chapter 3: Raman Spectroscopy (05 L)

Quantum theory of Raman effect, classical theory of Raman effect, pure rotational Raman spectra, vibrational Raman spectra, structure determination from Raman and IR spectroscopy. Ref. 1 Pages 111-128, 131-133, 138-141

Chapter 4: Electronic spectroscopy of molecules (08 L)

Electronic spectra of diatomic molecules. The Born Oppenheimer approximation, vibrational course structure, The Franck Condon principle, dissociation energy and dissociation products, rotational fine structure of electronic -vibration transitions, the Fortrat diagram, pre dissociation, ultraviolet photo electron spectroscopy, x-ray photoelectron spectroscopy.

Ref. 1 Pages 181-195, 227-231

Chapter 5: Mossbauer Spectroscopy (05 L)

Principle, instrumentation, Applications- chemical shift, quadrupole effect, effect of magnetic field. Ref:-1 Pages 323-332

References:

1. Fundamentals of molecular spectroscopy by Colin N. Banwell and Elain M. McCash. 5th Editon.
2. Physical chemistry by G.M. Barrow, 5th edition , 2006, Mc Graw Hill Education
3. Principals of Physical chemistry by Puri Sharma Pathania, 48th edition, Vishal Publishing Co.

4. Physical chemistry by Peter Atkins, Julio De Paula, 11th Edition , 2018, Oxford University Press

Course Outcomes

CO1: Remember basic concepts of molecular spectroscopy, selection rules, intensity of spectral lines and width of spectral transition.

CO2: Understand principles and applications of rotational, vibrational, raman, electronic and mossbauer spectroscopy.

CO3: Apply various spectroscopic techniques for gaining insights into molecular structure

CO4: Analyse vibrating diatomic molecule, simple harmonic and anharmonic oscillator, Scattering of light and Raman Spectrum.

CO5: Evaluate bond length, vibrational frequency, force constant and dissociation energy using spectral data.

CO6: Create awareness about rotational fine structure, vibrational coarse structure, Quadrupole effects

CHE-552: Inorganic Chemistry-II (4 Credits, 60 L)

(Coordination and Bioinorganic Chemistry)

SECTION-I: Coordination Chemistry (2 Credits, 30 L)

Chapter-1. Concept and Scope of Ligand Fields (06 L)

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

Chapter-2. Ligand Field Theory of Coordination Complexes (08 L)

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.

Chapter-3: Electronic spectra of Transition Metal Complexes (08 L)

Introduction, band intensities, band energies, band width and shapes, transition metal spectra of 1st, 2ndand 3rd 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.

Chapter-4: Magnetic Properties of Coordination Complexes (08 L)

Origin magnetism, types of magnetism, Curie law, Curie-Weiss Law, Magnetic properties of Complexes-Para magnetism, 1stand 2nd Ordered Zeeman effect, quenching of orbital angular momentum by Ligand fields, Magnetic properties of A, E and T ground terms in complexes, spin free and spin paired equilibria, temperature dependence of magnetism.

Reference

1. Ligand Field Theory and Its Applications by B.N. Figgis and M.A. Hitachman (Wiley India Pvt Ltd, 12 October 2010)
2. Symmetry and Spectroscopy of Molecules by K. Veera Reddy, Second Edition 2009: (New Age International Publication)
3. Elements of Magnetochemistry by R. L. Datta and A. Syamal, Second Edition

Course Outcomes: At the end of course student should able to –

CO-1: Define R. S. term, configuration, microstate, paramagnetic, diamagnetic ferromagnetic, antiferromagnetic, Curie and Neel temperature.

CO-2: Identify complex ions showing same R.S. terms, degeneracy of ground state terms ofmetal ions, and spin multiplicities of different configurations.

CO-3: Interpret electronic spectra for spin allowed Oh and Td complexes using Orgel diagram,Magnetic properties of A, E and T ground terms in complexes and selection rules.

CO-4: Calculate frequencies of absorption spectrum, 10Dq, Racah and nepholauxetic parameter for a complex, and magnetic moments of complexes

CO-5: Construct microstate table for various configuration and prepare correlations diagram and Tanabe-Sugano diagram for various configurations in Td an Oh ligand field.

CO-6: Assess appropriate full spectroscopic terms for various configuration/ion/term.

SECTION-II: Bioinorganic Chemistry (2 Credits, 30 L)

Chapter-1: Introduction of Bioinorganic Chemistry (04 L)

Historical Background and current relevance, role of Cu, Fe, Mn and Mo in metalloprotein, and metalloenzymes, Metals in medicine. Ref-1-Page No.1-19.

Chapter-2: Role of Inorganic Chemistry in Bioinorganic Research Thermodynamic Aspect (09 L)

HSAB concept, chelate effect and Irving-William series, pKa 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. Ref-1 Page No. 21-41.

Chapter-3: Functions and Transport of Alkali and Alkaline Earth Metal Ions (07 L)

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+; Ref-1: Page No. 152-171.

Chapter-4: Choice, Uptake and Assembly of Metal-Containing Units in Biology (05 L)

Bioavailability of metal ions, Enrichment strategies and intracellular chemistry of low abundance metal, Spontaneous self-assembly of metal cluster (FeS cluster) Ref-1: Page No. 103-125.

Chapter 5: Miscellaneous Topics of Bio-Inorganic Chemistry (05 L)

(a) Ca in Blood coagulation. Ref-4 (b) Magnesium in Photosystem I Ref-2 Page No. 67-75 and Ref-3 311-321 (c) Manganese in Photosystem II Ref-2 Page No. 67-75 and Ref-3 311-321 (d) Iron in Ferritin, Transferrin, Porphyrin based system. Ref-3 Page No. 247-277 (e) Zinc Finger protein, Calmodulin, Mercury detoxification; Ref-1 and 3

References:

1. Principles of Bioinorganic Chemistry by S.J. Lippard and J. M. Berg

2. Bioinorganic Chemistry: Inorganic Elements in Chemistry of Life by W.Kaim and B. Schwederski. 2nd Edition
3. Biological Inorganic Chemistry by Robert R. Crichton, 2nd Edition
4. Mikaelsson, M. E. (1991). The Role of Calcium in Coagulation and Anticoagulation. Coagulation and Blood Transfusion, 29– 37. doi:10.1007/978- 1-4615-3900-1_3

Course Outcomes: At the end of course student should able to –

CO-1: Define metalloproteins, metallo-eznymes, photosynthesis, HSAB concept, nucleic acids, metalloregulation, Biopolymer effects and acetylcholine receptor.

CO-2 : Explain chelate effect and Irving-William series, pKa values of coordinated ligands,Tuning of redox potential, and Reactions of coordinated ligands.

CO-3: Describe Fe-S clusters, model compounds and spontaneous self-assembly, metals inmedicine, blue copper proteins, and cytochromes, and Na/K pumps.

CO-4: Express nitrogen fixation, detoxification of mercury, structure of RNA, cis-platin, amino acids, siderophore,and calmoduline zinc finger proteins.

CO-5: Distinguish between hemoglobin and myoglobin, transferrin and ferritin, photosystem-I and photosystem-II.

CO-6: Decide role of metals in biological system, medicine, blood coagulation, oxygen storage and transport, photosynthesis and uptake and transport of iron

CHE-553, Organic Chemistry-II (4 credits, 60 L)

(Pericyclic Reactions, Molecular Rearrangements, Photochemistry and Organic Spectroscopy)

Section-I-Pericyclic Reactions and Molecular Rearrangements (2 credits, 30 L)

Chapter-1: Pericyclic reactions (16 L)

Electrocyclic, cycloaddition reactions, FMO approach, analysis by correlation diagrams, sigmatropic reactions, ene reactions, 1,3-dipolar additions.

Problem solving

Chapter-2: Molecular Rearrangements (12 L)

Mechanism to nucleophilic, electrophilic, and free radical molecular rearrangements, migratory aptitude

Carbon-carbon rearrangements: Pinacol-Pinacolone, Favorskii, Wolff and Benzil-Benzilic acid rearrangements

Carbon-nitrogen rearrangements: Hoffmann, Curtius, Lossen, Schmidt and Beckmann rearrangements.

Carbon-oxygen rearrangements: Bayer-Villiger rearrangement, Dakin oxidation

Oxygen-Carbon rearrangement: Fries rearrangement

Problem solving

Section-II- Photochemistry and Organic Spectroscopy (2 credits, 30 L)

Chapter-1: Photochemistry (12 L)

Principles of photochemistry, Jablonski diagram, photosensitization, photo-enolization, photochemistry of carbonyl and aromatic compounds, photo rearrangements, Paterno-Buchi Reaction, Barton reaction

Chapter-2: Organic Spectroscopy (18 L)

UV and IR Spectroscopy:

Calculation of λmax of aromatic system, Solvent effects, Factors affecting stretching frequencies and functional group interpretation from IR spectra, problems based on IR

^{1}H-NMR:

Principle, chemical and magnetic non-equivalence, chemical shifts and factors influencing chemical shift, chemical shifts of acidic protons, D2O exchange, spin-spin splitting, multiplicity patterns and coupling constant, Pascal's triangle, temperature dependent NMR.

^{13}C NMR:

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

Combined problems: Combined problems based on UV, IR and ^{1}H-NMR should be solved.

References

Essential books

1. Pericyclic Reactions by Ian Fleming, 2nd edition, Oxford.
2. Photochemistry and Pericyclic Reactions by Jagdamba Singh and Jaya Singh, 4th Edition, New Age International Publishers
3. Pericyclic Reactions: A Mechanistic and Problem-Solving Approach by Sunil Kumar Vinod Kumar S.P. Singh, 1st edition, Academic Press.
4. Mechanism and Structure in Organic Chemistry by E.S. Gould, 1st Edition, Holt, Rinehart and Winston of Canada Ltd.
5. Organic Chemistry, Jonathan Clayden, Nick Geeves, Stuart Warren, 1st Edition, Oxford University Press
6. Strategic Applications of Named Reactions in Organic Synthesis by Laszlo Kurti, Barbara Czako, 1st Edition, Academic Press
7. Reactions, Rearrangements and Reagents by S.N. Sanyal, 4th edition Bharati Bhawan Publishers.
8. Introduction to Spectroscopy by Donald L. Pavia Gary M. Lampman George S. Kriz James R. Vyvyan, 3rd Edition.
9. Spectrometric identification of organic compounds by R. M. Silverstein, F. X. Webster, 6th Edition, John Wiley and Sons.

Further reading

1. Conservation of orbital symmetry by R. B. Woodward and R. Hoffmann, Verlag chemie, weinheim (1970).
2. Orbital Symmetry: A problem solving approach by R. E. Lehr and A. P. Marchand; Academic (1972).
3. Organic reactions and orbital symmetry by T. L. Gilchrist and R. C. Storr; Cambridge, 2nd Edition, University Press.
4. Organic Photochemistry by Robert O. Kan, McGraw-Hill
5. Principles of Organic Synthesis by R.O.C. Norman and J.M. Coxon, 3rd Edition.

6. Spectroscopic methods in organic chemistry by D. H. Williams and I. Fleming, McGraw-Hill
7. Spectroscopy of Organic Compounds by P.S. Kalsi, 7th Edition, New Age International Private Limited.
8. Organic Spectroscopy: Principles and Applications by Jag Mohan, Narosa

Course Outcome: Student will able to –

CO1: Understand the concepts of pericyclic and photochemical reactions, and molecular rearrangements

CO2: Learn concepts of Organic Spectroscopy.

CO3: Identify the type of pericyclic and photochemical reactions

CO4: Solve the problems based on pericyclic and photochemical reactions and molecular rearrangements

CO5: Deduce the structure from the spectral data and justify the findings.

CO6: Develop problem solving ability of the students.

CHE- 554, Physical Chemistry Practical II [2 Credits, 60 L]

Part-I: Conductometry: (Any three)

1. Hydrolysis of NH_4Cl or CH_3COONa or aniline hydrochloride.

2.Determination of λ_0 or λ_∞ 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 $Pb(NO_3)_2$ with $K_2Cr_2O_7$.

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 H_2O

11.Estimation of halide in mixture.

12.Determination of composition of Zinc ferrocyanide complex by potentiometry

Part-IV: pH metry (Any two)

13.Determination of the acid and base dissociation constant of an amino acid and hence the isoelectric point of the acid.

14.Determination of dissociation constants of tribasic acid (phospheric acid)

15. 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)

16.Analysis of powder XRD of $SrTiO_3$ and Ag metal or any two compounds (Calculation- d, lattice constant, crystal volume and density, and assigning planes to peaks using JCPDS data)

17.Cyclic voltamogram of $K_3Fe(CN)_6$ in KCl/H_2O / Ferrocene in TEAP//MeCN

18.Detailed interpretation of Raman spectra of diatomic molecules.

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. 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, 7^{th} Edition, 2003.

5. Physical chemistry by Wien (2001)

6. Advanced Physical Chemistry Experiment, Gurtu and Gurtu, Pragati Publication (Meerut)

Course outcomes:

CO1: Students will grasp the fundamental principles of Conductometry, Polarography, Potentiometry and pH metry.

CO2: Students will familiar with the operation of Conductometer, Polarimeter, Potentiometer and pH meter.

CO3: Students will understand the concepts of conductance, resistance and learn how to calculate and interpret these values.

CO4: Students will learn to interpret polarographic waves and understand their significance in identifying electroactive species and determining their concentration.

CO5: Students will explore the applications of Potentiometry in various fields such as acid-base titrations, determination of pH and analysis of ionic concentration

CHE-555: Inorganic Chemistry Practical-II (2 Credits, 60 L)

Part-I: Synthesis of Coordination Complexes (Any three) (Ref. 2)

1. Synthesis and Purity Chloropentaamminecobalt(III) chloride.
2. Synthesis and Purity Nitro pentaamminecobalt(III) chloride.
3. Synthesis and Purity Bis[TrisCu(I)thiourea]
4. Synthesis of Cis and Trans $[Cu(gly)_2\ H_2O]$ (Ref. 8)
5. Synthesis and purity of $K_3[Mn(C_2O_4)_3].3H_2O$ (Ref-2)

Part-II: Inorganic Conductometry (Any two)

6. Structural determination of metal complexes by conductometric measurement – conductometric measurement of $[Co(NH_3)_6]Cl_3$, $[Co(NH_3)_5]Cl_2[Co(NH_3)_4]Cl$ and prediction of number of ionisable chlorides. (Ref-3).
7. To study complex formation between Fe(III)with sulfosalicylic acid by conductometry (Ref- 3).
8. To verify the Debye Huckel theory of ionic conductance for strong electrolytes KCl (1:1 type), $BaCl_2$ (1:2 type), K_2SO_4 (2:1 type) and $[K_3Fe(CN)_6]$ (3:1 type). (Ref-3)

Part-III: Inorganic Characterization Techniques (Any two)

9. Determination of equilibrium constant of M – L systems Fe(III)– Sulphosalicylic acid or Fe(III)–β–resorcilic acid by Mole ratio method **or any other M-L system** (Ref.-3, 5)
10. Solution state preparation of $[Ni(en)_3]S_2O_3$, $[Ni(H_2O)_6]Cl_2$, $[Ni(NH_3)_6]Cl_2$. 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)
11. 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)

12. Synthesis and photochemistry of $K_3[Fe(C_2O_4)_3].3H_2O$. (Ref-4)
13. Kinetics of substitution reaction of $[Fe(Phen)3]^{2+}$ (Ref-3)
14. Kinetics of formation of Cr(III)-EDTA complex (Ref-3)

Part-V: Ion – Exchange Chromatography (Any one) (Ref. 1 and 3)

15. Separation of mixture of Zn(II) and Mg(II) using Amberlite IRA 400 anion exchanger andquantitative estimation of separated ions Zn(II) and Mg(II)
16. Determination of anion exchange capacity of anion exchange resin.

Part-VI: Solvent Extraction and Calorimetry (Any one) (Ref. -1 and 3)

17. Determination of Cu(II) by solvent extraction as Dithiocarbamate complex
18. Determination of iron by solvent extraction techniques in a mixture of Fe(III) +Al(III) or Fe(III) + Ni(III) using 8–hydroxyquinoline reagent.

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. Vogel's Textbook of Inorganic quantitative analysis A.I. Vogel 4th Edn. (1964).
2. Experimental Inorganic Chemistry, MounirA. Malati, Horwood Seriein Chemical Science (Horwood publishing,Chichester) 1999.
3. Experiments in Chemistry, D. V. Jahagirdar, Himalaya Publishing House
4. General Chemistry Experiments,Anil. J Elias, University Press (2002)
5. Practical Physical Chemistry, B. Vishwanathan and P. S. Raghwan, Viva Books (2005)
6. Practical Inorganic Chemistry; Preparations, reactions and instrumental methods by Geoffrey Pass , Haydn Sutcliffe
7. Geoffrey Pass, Second Edition, 1974 Geoffrey Pass and Haydn Sutcliffe, Originally published by Chapman and HalI in 1974.
8. Synthesis of Cis [$Cu(gly)_2$ H_2O], trans [$Cu(gly)_2$], and Cis-$Ni(gly)_2(H_2O)_2$ and their characterization using thermal and spectroscopic techniques – A capstone inorganic laboratory, Journalof Chemical Education, https://doi.org/10.1021/acs.jchemed.9b00631

Course Outcome: Student will able to

CO-1: Define coordination complex, cell constant, resistance, specific conductance, equilibrium constant, absorbance, Beer's law, solubility product, chromatography, etc.

CO-2: Discuss photochemistry of potassium trioxalatoferrate complex, kinetics of formation of Cr(III)-EDTA, Determination of Cu(II)and Fe (II) by solvent extraction technique.

CO-3: Outline the flow-chart for synthesis of [Mn(acac)3], Chloropentaamminecobalt(III) chloride, Nitro pentaamminecobalt(III) chloride, Bis[TrisCu(I)thiourea complexes.

CO-4: Estimate purity of the [$Mn(acac)_3$], Chloropentaamminecobalt(III) chloride, Nitro pentaamminecobalt(III) chloride, Bis[TrisCu(I)thiourea complexes.

CO-5: Determine equilibrium constant of M – L systems Fe(III)–Sulphosalicylic acid, magnetic susceptibility (χg and χm) of mercury tetracyanato cobalt or Fe(acac) and magnetic susceptibility (χg and χm) of mercury tetracyanato cobalt or Fe(acac).

CO-6: Calculate the quantity from observation of the experiments and Interpret the result obtained respective experiments.

CHE-556, Organic Chemistry Practical II (2-Credits; 60 L)

(Single stage preparations with spectral analysis and Two stage preparations)

A. Single stage preparations and spectral analysis of the product (Any six)

1. Vanillin to Vanillyl alcohol
2. O-phenylenediamine to Benzotriazole
3. Ethyl acetoacetate to 1-phenyl-3- Methylpyrazol-5-one
4. Benzil to Quinoxaniline
5. Diels alder reaction of anthracene and maleic anhydride
6. Glycine to Hipuric acid
7. Synthesis of Cinnamic acid using Perkin's reaction
8. Synthesis of 2,6-Dicyanoaniline
9. O-phenylenediamine to 2-Methyl benzimidazole
10. p-Nitro Benzyl cyanide to p-Nitro Phenyl acetic acid

B. Two stage preparations (Any four)

1. Acetophenone → Benzalacetophenone → Epoxide
2. Benzoin → Benzil → Benzilic acid
3. Resorcinol → 4-methyl-7-hydoxycoumarin → 4-methyl-7-acetoxycoumarin
4. Cyclohexanone → Phenyl hydrazone → 1, 2, 3, 4-Tetrahydro carbazole
5. Phthalic anhydride → Phthalimide → Anthranilic Acid
6. Benzyl cyanide → p-Nitrobenzyl cyanide → p-Nitro phenyl acetic acid
7. Phthalimide → N-Benzylphthalimide → Benzylamine
8. O-Nitroaniline → O-Phenylenediamine → Benzimidazole

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 Task Force Committee, DST
3. Practical Organic Chemistry by Mann and Saunders, 4th edition, Pearson Education.
4. Vogel's Textbook of Practical Organic Chemistry, 5th edition Pearson India.

5. The synthesis, identification of organic compounds –Ralph L. Shriner, Christine K.F. Hermann, Terence C. Morrill and David Y. Curtin
6. Solvent-free Organic Synthesis by Koichi Tanaka.

Course Outcome: Student will able to -

CO1: Understand the theoretical concepts behind organic synthesis.

CO2: Acquire the experimental skills for separation, purification, identification and synthesis of organic compounds.

CO3: Design experimental set up for performing the organic reactions.

CO4: Monitor the organic reactions and analyse the products using spectral results.

CO5: Describe the mechanistic aspects of organic reactions.

CO6: Develop problem solving ability.

Chemistry Electives

(Any one option from the following four courses)

CHE-557(A), Organometallic Compounds and Inorganic Reaction Mechanism (2 Credits, 30L)

Chapter-1: Synthesis, Structure, Bonding and Applications of Organometallic Compounds (15 L)

Introduction to Organometallic Compounds, 18-Electron Rule and EAN rule, Metal carbonyl: preparation and properties, Polynuclear carbonyl: Structures, Carbonylate ions/Anionic carbonyl complexes: Isoelectronic and isostructural carbonyl and carbonylate ions, carbonyl Hydrate ions, Metal alkyls, Carbenes, carbynes and carbides, alkyls complexes, Metallocene containing four, five, six, seven, and eight membered ring, Synthesis, Bonding and structures of cyclopentadienyl complexes. Spectral analysis and characterization of organometallic complexes: IR and NMR, examples, Applications of organic metallic compounds: Hydroformylation, Monsanto acetic acid process, Wacker Process, Hydrogenation by Wilkinson's catalyst, Olefin metathesis, heterogeneous catalysis: Ziegler Natta Polymerization, Water gas reduction (Reference-1. Page No: 573-630, Reference-2 Page No: 475- 547).

Chapter-2: Inorganic Reaction Mechanism (15 L)

Introduction, background of Inorganic reaction mechanism Inert and labile compounds, Substitution reaction in square planner complexes, Rate law for Nucleophilic substitution reaction in square planner complexes, Trans effect and trans directing series, Stereochemistry of reactions: substitution in trans complexes, substitution in cis complexes Mechanism for Nucleophilic substitution reaction in square planner complexes, kinetics of octahedral substitution, Ligand field effect and reaction rates, Mechanism of substitution reaction in octahedral complexes, Reaction rates influenced by acids and bases, racemization and isomerization, Mechanism of redox reaction: Outer sphere mechanism and Inner sphere mechanism. Reaction of coordinated ligands: Hydrolysis of ester, Amides and peptides (Reference 1, Page no: 542-568)

References

1. Inorganic Chemistry: Principles of structure and reactivity by James E. Huheey 4th Edition.
2. Inorganic Chemistry by Gary L. Miessler, Paul J. Fischer and Donald A. Tarr 5th

Edition.

Course Outcomes: At the end of course student should able to -

CO1: Define various terms in organometallic chemistry and inorganic reaction mechanism etc.

CO2: Explain/Discuss various reaction mechanisms such as ligand insertion, inner and outersphere mechanism, ligand substitution reaction.

CO3: Discuss 1. Structure and bonding in carbonyl and organometallic complexes, 2: Trans effect, 3. Ligand field effects, catalytic cycles, 4. Inert and labile complexes, 5. Synthesismethods of organometallic compounds, etc.

CO4: Apply 18 electron rule. Applications of organometallic compounds and mechanism of these reactions.

CO5: Demonstrate IR spectra of carbonyl complexes, deduce structure of carbonyl complexes

CO6: Justify structures of organometallic compounds from spectral data

CHE-557 (B), Material Characterization Techniques (2 credits, 30 L)

Chapter-1: X-Ray Diffraction Methods (08 L)

Miller and Weiss indices, X-Ray Radiation, 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)

Chapter-2: Transmission Electron Microscopy (06 L)

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.

Chapter-3: Scanning Electron Microscopy (06 L)

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.

Chapter-4: X-Ray Spectroscopy for Elemental Analysis (10 L)

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, Analysing Crystal, Wavelength Dispersive Spectra, Energy Dispersive Spectroscopy, Detector, Energy Dispersive Spectra, Advances in Energy, Dispersive Spectroscopy, XRF Working Atmosphere and Sample Preparation, Energy Dispersive Spectroscopy in Electron Microscopes, Special Features, Scanning Modes, Qualitative and Quantitative Analysis, Qualitative Analysis, Quantitative Analysis, Quantitative Analysis by X-Ray Fluorescence, Fundamental Parameter Method, Quantitative Analysis in Electron Microscopy, Numerical.

References

1. Elaine A. Moore, Lesley E. Smart - Solid State Chemistry - an Introduction. Fourth Ed. CRC Press (2012)
2. YangLeng, Materials Characterization -Introduction to Microscopic and Spectroscopic Methods, Second Ed. Wiley-VCH,
3. R. D. Braun, Introduction to Instrumental Analysis, Second Ed.

Course Outcome: Student will able to –

CO1: Students are able to understand different characterization techniques of solids

CO2: Discuss Principle of XRD, instrumentation of powder XRD, Brags law, applications of XRD for crystal structure determination, numerical problems

CO3: Apply their knowledge to the interpretation of SEM and TEM images.

CO4: Differentiate between Scanning and Transmission of electron.

CO5: Explain the basics of X-rays, the Principle of XRF, types of XRF, instrumentation, qualitative and quantitative analysis, and numerical analysis.

CO6: Applications of different characterization techniques

CHE-557 (C) Green Chemistry [2 Credits, 30 L]

Chapter 1: Introduction to Green Chemistry (10 L)

What is Green Chemistry? Need for Green Chemistry. Goals of Green Chemistry. Problems in the applications of the goals of Green Chemistry. The 12 Principles of Green chemistry: application of principles, examples based on 12 principles. Environmentally benign solutions: Organic solvents and volatile organic compounds, solvent free systems, super critical fluids-supercritical carbon dioxide and supercritical water.

Chapter 2: Green Reactions: Case Studies (12 L)

1. Green Synthesis of the Compounds: Adipic Acid and Ibuprofen
2. Microwave assisted reactions: Oxidation of alcohols; Diels-Alder reaction in Organic Solvent (Atom economy) and Water (Green Solvent and Atom economy).
3. Ultrasound assisted reactions: Simmon-Smith Reaction
4. Enzymatic Inter esterification for production of no Trans-Fats and Oils.
5. Vitamin C synthesis –enzyme routes
6. Polythene manufacture-metallocene catalysis
7. Surfactants for carbon dioxide.

Chapter 3: Future Trends in Green Chemistry (08 L)

Renewable raw materials, Reagents and catalysts; multifunctional reagents; Combinatorial green chemistry; Click Chemistry, Solventless reactions; Solid Phase synthesis, Applications of Green chemistry in Sustainable Development

References

1. Green Chemistry - Theory and Practical by P.T. Anastas and J.K. Warner, Oxford University Press (1998).
2. Introduction to Green Chemistry by A.S. Matlack, Marcel Dekker (2001).
3. Real-World cases in Green Chemistry by M.C. Cann and M.E. Connely, American Chemical Society, Washington (2000).
4. Introduction to Green Chemistry by M.A. Ryan and M. Tinnes, American Chemical Society, Washington (2002).
5. Green Chemistry: An Introductory Text by M. Lancaster, RSC Publishing, 2nd Edition, 2010.

Course Outcomes: At the end of the course students will be able to-

CO1: Apply the principles of green chemistry to chemical processes.

CO2: Apply the principles of green chemistry to reduce the cost of chemical processes.

CO3: Develop economical synthetic route involving principles of green chemistry.

CO4: Analyze chemical data and choose safer and renewalbe raw materials for chemical processes.

CO5: Develop processes in accordance with Sustainable Development Goals.

CHEOD-557 (D) Nuclear and Radiation Chemistry [2 Credits, 30 L]

Chapter 1: Radioactivity (06 L)

Types of radioactive decay, general characteristics of radioactive decay, decay kinetics general expression for the activity of a daughter nuclide, Geiger- Nuttalls law, α- decay, A problem in classical physics, Internal conversion and the Auger effect. Ref:-1 Pages 101-109, 122-126, 151-154

Chapter 2: Elements of radiation chemistry (06 L)

Interaction of radiation with matter, interaction of Gamma radiation with matter, units for measuring radiation absorption, radiation dosimetry, radiolysis of water, free radicals in water, radiolysis of some aqueous solutions.

Ref 1: Pages 368-371, 377-384

Chapter 3: Nuclear fission. **(08 L)**

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

Ref 1: 209-224, 228-229

Chapter 4: Application of Radioactivity (10 L)

Typical reaction involved in preparation of radio isotopes- Szillard – Chalmer reaction, Radiochemical principles in the use of tracers, isotopes in elucidation reaction mechanism and structure determination, solubility of 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 measurement and control, friction and wear out, Gamma radiography

Ref 1: Pages 313-318, 320-334, 338-342, 350-352, 357-359

References:

1) Elements of nuclear chemistry by H. J. Arnikar (revised 4th edition)
2) Chemical applications of radioisotopes by H.J.M. Brown. (1 June 1969)
3) Source book of atomic energy by S. Glasshone Krieger Publishing Company; 3rd edition (1 January 2012)

Course Outcomes

CO1: Remember basic concepts of radioactive decay, decay kinetics and Interaction of radiation with matter.

CO2: Understand concepts of nuclear and radiation Chemistry, radiolysis of water, the process of nuclear fission and fission fragments.

CO3: Nuclear chemistry applications: reaction mechanism, medical treatment, isotopic labelling, and carbon dating.

CO4: Study units for measuring radiation absorption, interaction of γ radiation with matter and radiation dosimetry.

CO5: Use proper isotopic notation to write down and balance a nuclear reaction. State and compare the differences and similarities between a nuclear change and a chemical change.

CO6: Identify and define various types of nuclear changes or processes including fission and decay reactions.

CHE-558, On Job Training/Internship (4 credits, 120 hours)

Students in this course will be required to do On the Job Training (OJT)/Internship in relevant industries/government sectors/institutes, etc. to gain practical training. As a prerequisite for OJT, the department may conduct necessary lectures/workshops/seminars. The course will be run as per the guidelines of the Institute /the University and Government of Maharashtra. Most of our graduates are expected to seek employment in industries, pursue teaching careers, or establish small enterprises after obtaining their M.Sc. degree. Therefore, the following options would be provided to the students to develop skilled and competent students.

a) Hands on Training on various analytical instruments- UV-Visible Spectrometer, Fourier Transform Infrared Spectrometer, Nuclear Magnetic Resonance Spectrometer, Mass Spectrometry, Gas Chromatography, HPLC, X-Ray Diffractometer, Powder X-ray Diffractometer, Thermal Analyzer (TGA-DSC), Scanning electron microscope, Transmission electron microscope, BET Surface Analyzer, Raman Spectrometer, CHN Analyzer

Note: Analytical instruments (from above list) should be selected for OJT that should complete 120 hours training.

OR

b) Teacher Training Course:

1) Development of MOOCS
2) Development of Learning Management System (LMS)

OR

c) Internship in Industry or National research laboratory.

OR

d) To develop Entrepreneurship, production of the following items, including packaging

1) Dye
2) Acids, caustic soda
3) Fire Extinguisher
4) Fertilizers
5) Any other industry material

OR

e) Field projects that are aligned with the Chemistry Subject.

A detailed report should be submitted for the evaluation of On Job Training/Internship.