

SHIVAJI UNIVERSITY, KOLHAPUR - 416004, MAHARASHTRA

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Estd. 1962 &A++" Accredited by NAAC (2021) With CGPA 3.52 शिवाजी विद्यापीठ, कोल्हापूर -४१६००४,महाराष्ट्र दूरध्वनी-ईपीएबीएक्स -२६०९०००, अभ्यासमंडळे विभाग दुरध्वनी ०२३१–२६०९०९४ ०२३१–२६०९४८७



SU/BOS/Science/346

Date: 24/06/2024

To,

he Head/Co-ordinator/Director
All Concerned Department (Science)
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Subject: Regarding syllabi of M.Sc. Part-II (Sem. III & IV) as per NEP-2020 (2.0) degree programme under the Faculty of Science and Technology.

Sir/Madam,

With reference to the subject mentioned above, I am directed to inform you that the university authorities have accepted and granted approval to the revised syllabi, nature of question paper and equivalence of M.Sc. Part-II (Sem. III & IV) as per NEP-2020 (2.0) degree programme under the Faculty of Science and Technology.

	M.ScPart II (Sem. III & IV) as per NEP-2020 (2.0)					
1.	Inorganic Chemistry	4.	Analytical Chemistry			
2.	Organic Chemistry	5.	Applied Chemistry			
3.	Physical Chemistry	6.	Industrial Chemistry			

This syllabus, nature of question and equivalence shall be implemented from the academic year 2024-2025 onwards. A soft copy containing the syllabus is attached herewith and it is also available on university website <u>www.unishivaji.ac.in NEP-2020(Online Syllabus)</u>

The question papers on the pre-revised syllabi of above-mentioned course will be set for the examinations to be held in October /November 2024 & March/April 2025. These chances are available for repeater students, if any.

You are, therefore, requested to bring this to the notice of all students and teachers concerned.

Thanking you,

Dy Registrar r. S. M. Kubal

Copy to:

1	The Dean, Faculty of Science & Technology	4	P.G Admission / Eligibility Section
2	The Chairman, Respective Board of Studies	5	Computer Centre/ Eligibility Section
3	B.Sc. Exam/ Appointment Section	6	Affiliation Section (U.G.) (P.G.)



Shivaji University, Kolhapur

M.Sc. Part-II Inorganic, Organic, Physical, Analytical, Applied and Industrial Chemistry Syllabus

as per

National Education Policy 2020

(NEP 2.0)

To be implemented from June- 2024-25

Applicable for University Department and Affiliated Colleges PG Centres

Name of Program: M.Sc. Inorganic Chemistry

1. Program Outcomes (POs)

PO1: Students will have a thorough knowledge in the fundamentals and application of modern chemical and scientific theories including those in all branches of chemical sciences.

PO2: Students will be able to design and carry out scientific experiments as well as accurately record and analyse the results of such experiments.

PO3: Students will be able to use the evidence based comparative chemistry approach for synthesis and analysis of the chemical compounds.

PO4: Students will be skilled in problem solving, critical thinking and analytical reasoning as applied to scientific problems.

PO5: Students will be able to clearly communicate the results of scientific task in oral and written formats. Students will be able to function as a member of an interdisciplinary problem solving team.

PO6: Students will be able to explain the role of Inorganic Chemistry for addressing social, economic, and environmental problems.

2. Program Specific Outcomes (PSOs)

PSO1: The students will be able to get global level research opportunities to pursue Ph.D. programme, targeted approach of competitive Exams such as CSIR-NET/GATE/SET, discipline specific competitive exams conducted by service commission, etc.

PSO2: The students will be able to get employment opportunities in various industries like petrochemicals, metallurgical, materials and pharmaceutical, etc.

PSO3: Understands the background of Inorganic reaction mechanisms, complex chemical structures, and instrumental methods of chemical analysis, separation techniques and analytical methods of general purpose.

PSO4: Gains complete knowledge about all fundamental aspects of all the elements of chemistry.

3. Framework of NEP 2.0 as per NEP-2020 for M. Sc. Degree in Inorganic Chemistry

Class	SEM	Level	Mandatory Subject	Elective Choose any One	RM (4 Cr)	OJT/FP (4 Cr)	RP	Cumm. Cr	Degree
M.Sc. II	III	6.5	ICH.301 (4Cr)	E-ICH.304 (4Cr) OR			RP-ICH.	22	M.Sc. Degree
			ICH.302 (4Cr)	E-OCH.304 (4Cr) OR			306 (4 Cr)		in Analytical
			ICH.303 (4Cr)	E-ACH.304 (4Cr) OR E-ACH.304 (4Cr) OR					after 3/4 yr.
			PR-ICH305 (2 Cr)						UG
	IV	6.5	ICH.401 (4Cr)	E-ICH.404 (4Cr) OR			RP-ICH	22	
			ICH.402 (4Cr)	E-OCH.404 (4Cr) OR			405 (6 Cr)		
			ICH.403 (4Cr)	E-ACH.404 (4Cr) OR					
Cum. Cr.	For 1 Y Degree	ear PG	26 Cr	8 Cr			10	44	

3. Course Structure: M.Sc. Part-II, Inorganic Chemistry

Semester - III

Major Mandatory

Course Code	Course Title	Credits
ICH301	Inorganic Chemical Spectroscopy	4
ICH302	Coordination Chemistry – I	4
ICH303	Nuclear Chemistry	4
PR-ICH305	Practical Course	2
RP-ICH306	Research Project	4

Major Elective (Choose any one)

Course Code	Course Title	Credits
E-ICH304	Organometallic and Bioinorganic Chemistry	4
E-OCH304	Drug and Heterocycles	4
E-PCH304	Solid State Chemistry	4
E-ACH304	Environmental Chemical Analysis and Control	4

Semester - IV

Major Mandatory

Course Code	Course Title	Credits
ICH401	Instrumental Techniques	4
ICH402	Coordination Chemistry-II	4
ICH403	Chemistry of Inorganic Materials	4
RP-ICH405	Research Project	6

Major Elective (Choose any one)

Course Code	Course Title	Credits
E-ICH404	Energy and Environmental	4
	Chemistry	
E-OCH404	Applied Organic Chemistry	4
E-PCH404	Surface Chemistry	4
E-ACH404	Applied Analytical Chemistry	4

5. Detailed Syllabus

M.Sc. Part-II (Sem- III) Inorganic Chemistry

ICH301: Inorganic Chemical Spectroscopy

Unit I: Molecular Symmetry and Group Theory

Introduction to Symmetry, Symmetry operations, Symmetry elements, Point group and its classification (Cn-type, Dn-type, Special-type), Schoenflies symbol for point groups, Determination of point group for AB₂ (Bent), AB₃ (Trigonal pyramid), AB₃ (Trigonal Planar), AB₄ (Square planar), AB₅ (Trigonalbipyramidal), AB₆ (Octahedral), CO₂, HCl, CO, Ortho–, meta– & para–disubstituted benzene molecules. Symmetry and dipole moment of molecule, Symmetry and optical activity, Group and its Properties, Group multiplication table, Matrix representation of symmetry elements, Reducible and Irreducible representations, Character of a representation (character of matrix), Properties of Irreducible representation, Great orthogonally theorem (without proof) and its importance, Construction of character table for C_{2v} & C_{3v} point groups, Mulliken symbolism rules for irreducible representations & its illustrations, Direct product, Standard reduction formula.

Unit II: IR and Raman Spectroscopy

15 hrs.

A) Infrared spectroscopy: The vibrating diatomic molecule, The simple harmonic oscillator, The anharmonic oscillator, The diatomic vibrating rotator, Vibration– rotation spectrum of carbon monoxide, Breakdown of Born–Oppenheimur approximation, The vibration of polyatomic molecules, Overtones and combination frequencies, The influence of rotation of the spectra of polyatomic molecules, Techniques and Instrumentation, Applications.

B) Raman spectroscopy: Classical and Quantum theory, Pure rotational Raman Spectra, vibrational Raman spectra, Rule of mutual exclusion, Overtone and combination vibrations, Rotational fine structure, Outline of technique and instrumentation, Applications. Modes of vibrations, Selection Rules for Infrared and Raman Spectra, Normal modes of vibrations in AB₂ (Linear/Bent), AB₃, AB₄, AB₅, Octahedral AB₆ molecules with factors affecting band frequencies.

Unit III: Mass Spectroscopy:

Basic principle, Instrumentation, Electron-impact Induced and Fast Atom Bombardment (FAB) spectrometry, qualitative and semiquantitative theories including QET, concept of metastable ions transitions, Stevensons's rules. Applications to metal compounds containing carbonyl, alkyl, cyclopentadienyl and acetylacetonate.

Unit IV: NMR and X-ray Photo electron Spectroscopy

A) NMR Spectroscopy:

Principle Instrumentation of NMR, the chemical shift, mechanism of electron shielding and factors contributing to the magnitude of chemical shift. Local & remote effect, spin-spin splitting, applications of spin coupling to structural determination, double Resonance techniques. The contact and Pseudo contact shifts Factors affecting nuclear relaxation, an overview of NMR of metal nucleus with emphasis on ¹⁹⁵Ag &¹¹⁹Sn NMR, applications of solid-state NMR technique.

B) X-ray Photo electron Spectroscopy (XPS)

Introduction and basic theory, Instrumentation, sample selection and preparation, spectral analysis, Ar ion sputtering technique and applications of XPS.

Reference Books:

- 1. K. Burger, Coordination Chemistry-experimental methods, Butterworth's
- 2. R. Drago: Physical method in Inorganic Chemistry, DUSAP.
- 3. Hill & Day advanced methods in Inorganic Chemistry, J.Weily
- 4. F.A. Cotton, chemical application of group theory, Weily eastern
- 5. Figgis, Introduction to ligand field theory field
- 6. Schaefer & Gilman: Basic principles of ligand field Theory, J. Wiely
- 7. P.R. Backer: Molecular symmetry and Spectroscopy A.P.
- 8. Ferraro Ziomeek, Introduction to Group theory, plenum
- 9. Scotland Molecular symmetry DVN
- 10. Dorian: symmetry in Chemistry EWAP
- 11. Hall: Group theory and symmetry in Chemistry MGLt
- 12. Nakamoto Infrared R Raman Spectra of Inorganic & Coordination compounds J.Weily
- 13. Nakanisha: Spectroscopy and structure J. Weily
- 14. Ferroro: Metal ligand and related vibrations
- 15. CNR Rao Spectroscopy in Inorganic Chemistry Vol I, II, III

15 hrs.

8 hrs.

- 16. Durie: vibrations spectra and structure Vol. I to IV, Elsevier
- 17. Dudd, chemical Spectroscopy Elsevier
- 18. Popel: H.N.M.R. Spectroscopy J.Weily
- 19. R.J. Abraham, J.Fisher and P Loftus Wiley Introduction to NMR spectroscopy.
- 20. P.K. Bhattacharya: Group Theory & Its Chemical Applications
- 21. K.V. Reddy: Symmetry & spectroscopy of Molecules.
- 22. M. R. Litzow and T R Spelding, Mass Spectroscopy of Inorganic & Organometallic Compounds, Elsevier, 73.

Course Outcomes (COs):

CO1: At the end the student should be able to: Recognize symmetry elements in a molecule; State the point group a molecule belongs to; Combine matrices and set up matrix for transformations and acquisition of a theoretical support which underlies much of spectroscopy.

CO2: Able to describe molecular vibration with the interaction of matter with light, Explain the basic concepts in IR and Raman Spectroscopy, Examines IR and Raman spectroscopy and molecular structure determination by the simple molecules.

CO3: Students will be able to identify, describe and explain the function of the several components of a mass spectrometer and predict the fragmentation patterns expected.

CO4: The ability to investigate and determine the local structure of typical elements in inorganic compounds and able to explain the surface composition and chemical nature of the surface elements.

ICH302: Coordination Chemistry-I

Unit I: Metal-ligand bonding:

Crystal Field Theory: Splitting of d-orbital in tetragonal, square planar and trigonal bipyramid complexes. CFSE-factors affecting the magnitude of 10 Dq-evidence for crystal field stabilization, tetragonal distortion from octahedral symmetry, John teller effect, nephelauxetic effect. CFSE and their uses, factors affecting CFSE, Limitations of crystal field theory. M.O. theory for octahedral, tetrahedral and square planar complexes with and without π -bonding.

Unit II: Electronic spectra of Transition Metal complexes: 15 hrs.

Determining the Energy terms, Spin-orbit (L-S) coupling scheme, Hund's rule, Derivation of the term symbol for a d¹ to d⁹ configuration, electronic spectra of transition metal complexes-Laporte 'orbital' selection rule, spin selection rule. Orgel diagrams for octahedral metal complexes. Racah parameters, calculations of 10 Dq, B and β parameters for octahedral complexes of cobalt and nickel, Tanabe-Sugano diagrams for octahedral complexes, Charge transfer spectra, Selection rule and charge transfer spectra.

Unit III: Magnetic properties of Transition metal complexes: 15 hrs.

Types of magnetic behaviour, origin of paramagnetism, Spin-orbit interaction, Lande interval rule, Diamagnetism, Pascal constants, Ferromagnetism and antiferromagnetism of metal complexes; temperature dependent paramagnetism, Van Vleck's equation, Its derivation and applications, magnetic anisotropy, anamoulous magnetic moment, Quenching of orbital moment, Spin orbit coupling and magnetic moment, Determination of magnetic susceptibility. Spins crossover phenomenon.

Unit IV: Mixed Ligand complexes

Stabilities of ternary complexes, Dynamics of formation of ternary complexes reaction of Coordination ligand in ternary complexes, Mimicking reactions in biological systems, enzyme models, Amino acids ester hydrolysis, peptide synthesis & hydrolysis, Decarboxylation of βketo acids, Applications of mixed ligand complexes in catalysis.

Reference Books:

- 1. Jones: Elementary Coordination Chemistry. J. Weily
- 2. Graddon: Introduction to Coordination Chemistry. J. Weily

15 hrs.

3. Drago: Physical methods of Inorganic Chemistry. J. Weily.

- 4. Graddon: Introduction to coordination Chemistry, Parasmom
- 5. Lewis and Wilkins: Coordination Chemistry. J. Weily
- 6. Msrtel: Coordination Chemistry Vol I, II VNR
- 7. Earnshaw: Introduction to Magneto Chemistry
- 8. Mabbs & Machin Magnetism & transition metal complexes Chamman hall
- 9. Calvin, Magnetic properties of transition metal complexes.
- 10. L.N. Maley: Magneto Chemistry
- 11. Datta & Shymlal: Elements of Magneto Chemistry
- 12. Martel & Taqui Khan: homogeneous catalysis with metal complexes Vol.I & II AP.

13. James E. Huheey: Inorganic Chemistry Principles of Structure and reactivity, Harber and Row, Publishers Inc. New York 1972.

14. K.P. Purcell & J.C. Kote: An Introduction to Inorganic Chemistry Holt Sounders, Japan 1980.

15. William L. Jolly: Modern Inorganic Chemistry, Mecgrow Hill USA, 1984

16. F.A. Cotton & R.G. Wilkinson: Advanced Inorganic Chemistry

Course Outcomes (COs):

CO1: To be able to describe and explain the bonding in d-metal complexes using crystal field and ligand field theories and calculate the crystal field stabilization energy and its role in stabilizing the complexes.

CO2: At the end of the course students should be able to interpret simple electronic spectra and predict both position and intensity based on Orgel/Tanabe-Sugano diagrams and explain the spectroscopic properties of transition metal complexes.

CO3: Students should be able to estimate the spin-only magnetic moment for given complex and predict the nature of magnetic properties.

CO4: Students will be able to explain the reactivity and stabilities of ternary complexes and their reactions.

ICH303: Nuclear Chemistry

UNIT-I: Systematic of alpha, beta and gamma decays

Alpha decay, energy curve, spectra of alpha particles, Giger-Nuttal law, theory of alpha decay, penetration of potential barrier, beta decay, range of energy relationship, beta spectrum, sergeants curve, Fermi theory of beta decay, matrix elements, allowed and forbidden transitions, curie plots, gamma decay, Nuclear energy levels, selection rule, isomeric transitions, Internal conversion, Auger effect

UNIT-II: Nuclear Structure and Stability

Binding energy, empirical mass equation, The nuclear models, the liquid drop model, Single particle shell model, Fermi gas model & collective/lunified nuclear model, nuclear spin, parity & magnetic moments of odd mass number nuclei and numerical.

Unit III: Nuclear reactions and Nuclear fission

Introduction, Production of projectiles, nuclear cross section, nuclear dynamics, threshold energy of nuclear reaction, Coulomb scattering, potential barrier, potential well, formation of a compound nucleus, Nuclear reactions, direct Nuclear reactions, heavy-ion induced nuclear reactions, photonuclear reactions.

Liquid drop model of fission, fission barrier and threshold, fission cross section, mass energy and charge distribution of fission products, symmetric and a symmetric fission, decay chains and delayed neutrons

UNIT-IV: Reactor Theory and Applications of Radioactivity

Nuclear fission as a source of energy, Nuclear chain reacting systems, critical size of a reaction, research reactors, graphite moderated, heterogeneous, enriched uranium reactors, light water moderated, heterogeneous, enriched uranium reactors, water boilers enriched aq. Homogeneous reactors, Thermonuclear reactors, gamma interactions, shielding and health protection. Reactors in India, Tracer technique in the field of analytical chemistry structure determination elucidation of reaction mechanism, isotopic dilution analysis, neutron activation analysis applications in biological, medical, industrial fields, Age determination.

15 hrs.

15 hrs.

15 hrs.

Reference Books:

- 1. Friedlander, Kennedy and Miller, Nuclear and Radio Chemistry: John Wiley
- 2. B. G. Harvey, Nuclear Chemistry

3. Hassinsky: Translated by D. G. Tuck, Nuclear Chemistry and its application: Addison Wiley.

- 4. B.G. Harvey, Introduction to Nuclear Physics and Chemistry
- 5. Maeclefort: Nuclear Chemistry: D. Van Nostrand
- 6. An N. Nesmeyannoy: Radiochemistry: Mir
- 7. Jacobs et al: Basic Principles of nuclear Science and Reactors, V. Nost & EWAP
- 8. N. Jay: Nuclear Power Today Tomorrow: ELBS
- 9. Kenneth: Nuclear Power Today, Tomorrow: ELBS
- 10. Essentials of Nuclear Chemistry, W. J. Arnikar, John Wiley
- 11. Nuclear and Radiation Chemistry: B. K. Sharma, Krishna Publication
- 12. A Introduction to Nuclear Physics: R. Babber and Puri.
- 13. Essential of Nuclear Chemistry by H. J. Arnikar

Course Outcomes (COs):

CO1: Students will be able to different modes of radioactive decay and also theories of radioactive decay.

CO2: Students will be able to explain the nuclear structure and stability using various models.

CO3: Students will get basic knowledge of nuclear reactions, mechanism and energy calculations.

CO4: At the end students should be able to describe the fundamentals of nuclear reactors, isotopic chemistry, and the applications of radioactivity.

PR-ICH305 Inorganic Chemistry Practical (2 Cr.) 60 hrs.

A) List of Experiments:

- 1. Ore Analysis
- 2. Alloy Analysis
- 3. Preparation of coordination complexes
- 4. Separation and estimation of ions using ion exchange chromatography
- 5. Spectrophotometry
- 6. pH Metry

- 7. Nephelometry
- 8. Potentiometry
- 9. Conductometry
- 10. Spectro Fluorimetry
- 10. Thermal analysis

(Any other experiments may be added whenever required)

B) Interpretation exercises

- 1. X-ray powder diffraction analysis of cubic compound
 - a. Determination of lattice constants and geometry
 - b. Partical Size
 - c. Density
- 2. Interpretation of Mossbaur spectrum with reference to determination of a) isomer shiftb) quadruple splitting c) Internal magnetic field d) general comment
- Interpretation of IR spectrum with reference to stretching vibration 0-2 C=N, C=O, N-, M-O.
- 4. Interpretation of NMR spectrum with reference to calculation of chemical shifts and general comments.
- 5. Interpretation of absorption spectra for
 - a. Verification of position of ligands in spectrochemical series
 - b. Determination of geometry (Octahedral, Square planar, tetrahedral) of a given compound.
 - c. Calculation of spectral splitting parameters.
- 6. Interpretation of polar gram for determination of half wave potentials and unknown concentration.
- 7. Calculation of band gap of semiconductors with the help of plots of log Vs.10 $\frac{3}{4}$.

NOTE: Student should perform their practical work in the laboratory minimum 15 days in one semester for 2 credits.

RP-ICH306: Research Project

(4 Cr)

See Annexture-I for details.

M.Sc. Part-II (Sem- IV) Inorganic Chemistry

ICH401: Instrumental Techniques

Unit I: X-ray Diffraction Techniques

X-ray Sources (X-ray tube and synchrotron sources with their principle of working characteristics of emission spectrum), Bragg's law of diffraction, methods of diffraction (powder and single crystal), Powder diffraction: instrumentation, use of standards, characteristics of powder XRD pattern, significance of peak intensities, systematic absences of reflections, indexing of powder XRD pattern, determination of lattice parameters and solving cubic crystal structure using powder XRD data, qualitative (identification of the phases) and quantitative analysis (phase quantification), crystallite size determination, determination of relative % crystallinity. Single crystal diffraction: Advantages of single crystal diffraction over powder diffraction, introduction to Laue, rotation photograph and oscillation methods. Introduction to crystallographic database and file formats (raw data files, cif and pdf), Open source computer based crystal structure building and visualization tools.

Unit II: Mossbauer Spectroscopy

Principle of Mossbauer spectroscopy, Recoiless absorption and emission of gamma-rays, Doppler shift, Instrumentation, Isomer shift and its factors affecting, Quadruple splitting, Temperature Dependence of MB parameters, Zeeman Splitting (Six fingered MB lines), MB spectra of iron and tin compounds, Applications, Numericals.

Unit III: Electron Spin Resonance Spectroscopy

Principle of ESR Spectroscopy, Presentation of spectrum, Hyperfine splitting in some proton systems, Rules for evaluating ESR lines (Naphthalene anion radical, Pyrazine anion radical, Isomers of Xylene anion radicals, VO2+, Quinoline radical, Isoquinoline radical, Quinoxaline radical, Anthracene radical, Phenanthracene radical, Pyrene radical, Alkyl halide radicals, Quinone & Isoquinone anion radicals, nitrogen/deuterium containing radicals), Superhyperfine splitting, Instrumentation, 'g' value and factors affecting it, Zero field splitting, Karmers's degeneracy, Applications, Numericals.

15 hrs.

15 hrs.

Unit-IV: Advanced Instrumental Tools for Analysis of Inorganic materials 15 hrs.

Time resolved studies of chemical reactions such as material synthesis (solid state, hydrothermal, sol/gel, thin film growth etc., cathode/anode materials in lithium ion batteries during charge/discharge cycles, in situ X-ray diffraction methods for thermal expansion/contraction studies, structural studies as a function of temperature and pressure (XRD methods), Temperature programmed techniques (temperature programmed desorption/oxidation/reduction: TPD/TPR), methods of determination of surface acidity and basicity of solid catalysts, Computer softwares for plotting and analysis of the XRD data, Structure drawing softwares (VESTA)

Reference Books:

- Powder Diffraction Theory and Practice, Edited by R E Dinnebier and S J L Billinge, RSC publishing, 2008.
- 2. Catalysis, Principles and Applications, Editors: B. Viswanathan, S. Sivasanker, A.V. Ramswamy, Narosa Publishing House
- 3. VESTA 3 for three-dimensional visualization of crystal, volumetric and morphology data, K. Momma and F. Izumi (2011), J. Appl. Crystallogr., 44, 1272-1276.
- 4. Elements of X-ray Diffraction, B.D. Cullity, Second Edition, Addison Wesley, 1978. Neutron Scattering in Chemistry, Baun, G.E. Butleworth, London, 1971.
- 5. Mossbaur Spectroscopy, Greenwood N.N., Gibbs T.C., Chapmann Hall, 1971.
- Chemical Application of Mossbaur Spectroscopy, Goldanski V.I & Harber R.H., Academic Press 1968.
- 7. Spectroscopy in Inorganic Compounds CNR Rao & Ferraro G.R., Academic Press, 1970.
- 8. Basic Principles of Spectroscopy Cheney R.Mac Grows Hill, 1971.
- 9. Thermal Method, Wendlandt, W.W. John, Wiley, 1986.
- 10. Principles of Instrumental analysis, Skoog, III rd edn., Sounders, 1985.

Course Outcome (COs):

CO1: Students will obtain knowledge of the working principles involved for selective analytical methods and the fundamental basics of the instrumentation including electronic spectroscopy and diffraction techniques.

CO2: Students will understand the advanced methods involved in determination of the quality and quantity of chemical substances in given compounds.

CO3: At the end of the course students will learn the interpretation of the experimental data obtained using various techniques and instruments for laboratory analysis carried out for quality assurance.

CO4: Students will be able to demonstrate the use of complementary analytical techniques to define the system/materials more precisely. To know the recent advancements in the instrumental methods of temperature programmed analysis.

ICH402: Coordination Chemistry-II

Unit-I Reaction Mechanism of Transition Metal complexes-I 15 hrs.

Energy profile of reaction. Inert and labile complexes, interpretation of liability and inertness of transition metal complexes on the basis of VBT and CFT. Factors affecting the liability of a complex, transition state or activated complex, substrate, attacking reagents electrophilic and nucleophilic, Nature of central atom. Reactions of metal complexes, ligand substitution reaction, Kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct & indirect evidences in favour of conjugate mechanism, anation reaction.

Unit-II Reaction Mechanism of Transition Metal complexes-II 15 hrs.

Substitution reaction in square planer complexes: the trans-effect, Theories of Trans effect, uses of trans-effect, cis effect, Electron transfer reactions. Types of electron transfer reactions, conditions of electron transfer, and mechanism of one-electron transfer reactions, outer sphere and inner sphere mechanisms, two electron transfer reactions, complimentary and noncomplimentary electron transfer reactions. Marcus Theory, Cross reactions, Inner sphere Reactions, Recimization and isomerisation in transition metal complexes.

Unit-III Photochemistry

Absorption, excitation, photochemical laws and quantum yield, Electronically excited states and their life-time measurement, Electronically excited states of Metal complexes, type of photochemical reactions, substitutions reactions, rearrangement reactions, redox reaction, Photochemistry of Coordination compounds, LMCT states and MLCT states, Charge transfer spectra, charge transfer excitations, methods for obtaining charge transfer spectra.

Unit-IV Applications of Coordination Compounds

Metal Complexes in Analytical Chemistry Inorganic Qualitative Analysis, The 'brown ring' test, Complexometric Titrations, Complexes in Colourimetry, Coordination Compounds in Gravimetry, Stabilization of Oxidation States, Complexes in Separation of Metals. Metal Complexes in Medicinal Chemistry: Complexation in Food Poisoning, Metal Complexes in Therapy. Metal Complexes in Industrial Processes: Heavy Metals-protein Complexes in the Rasching Process, The Ziegler-Natta Catalyst, Metal complexes in alkene conversions, Complexes and Electroplating, Complexes in Metallurgy. Copper Metal dissolves in Aqueous Potassium Cyanide, Complexes in water softening, Metal complexes in Agriculture.

Reference Books:

- 1. R. Gopalan and V. Ramlingam: Concise Coordination Chemistry.
- 2. J. E. Huheey, Ellen A. Keiter and Okhil K. Medhi: Inorganic Chemistry: Principle of Structure and Reactivity.
- 3. K. F. Purcell, J. C. Kotz: An Introduction to Inorganic Chemistry.
- 4. F. Basolo and R. Pearsons: Mechanism of Inorganic Reactions: A Study of Metal Complexes in Solution.
- 5. Obe, M. L. Inorganic reaction mechanism, Nelson, London, 1972.
- 6. Taube, electron transfer reactions of metal complex ions in solution. Academic Press, 1970
- 7. E. S. Gould, Inorganic Chemistry.
- V. Balzani and V. Cavassiti, Photochemistry of coordination compounds, AP, London, 1970.
- 9. K. Burger, Coordination Chemistry Experimental methods, Butterworths.
- 10. K. K. Rastogi and Mukharjee, Fundamentals of photochemistry, Wiley eastern.
- 11. J. G. Calverts and J. N. Pits, Photochemicals of Photochemistry, John Wiley.
- 12. Wells, Introduction to Photochemistry.
- K. M. Macky, R. A. Macky, Modern Inorganic Chemistry, 4th edn., Blackie, London 1989.
- B. R. Puri, L. R. Sharma, K. C. Kalia, Principles of Inorganic Chemistry, Vallabh Publications, Delhi, 2005.

Course Outcome (COs):

CO1: After successful completion of the course students will be able to familiar with various reactions of transition metal complexes and will be able to predict the mechanism involved using direct and indirect evidences.

CO2: At the end students will be able to explain the cis-effect, trans-effect, and mechanism of electron transfer reactions.

CO3: Students will be able to explain the photochemistry of transition metal complexes.

CO4: Students will be able to describe the industrial applications of transition metals as catalysts.

ICH403: Chemistry of Inorganic Materials

Unit-I: Solid State Materials

15 hrs.

A) Bonding in crystals, Crystal systems and Bravais Lattice, Lattice planes and their designation. Metallic Crystal structures: Face-centered cubic (fcc), body-centered cubic (bcc), hexagonal close-packed (hcp) structure. Radius ratio rule (2, 3,4,6,8 co–ordinate structures), octahedral and tetrahedral voids. Isomorphism and polymorphism, Numericals.

B) Simple type structures:

AB type: NaCl, CsCl, Zinc sulphide (sphalerite or cubic and hexagonal), AB₂ type: Fluorite (CaF₂), TiO₂(Rutile), CdCl₂, CdI₂ structures, AB₃ type: ReO₃, BiI₃, A₂B₃ type: Corundum Al₂O₃, α -Fe₂O₃, Mn₂O₃, ABO₃type: Perovskite Structures (Barium titanate, lead titanate, CaTiO₃, FeTiO₃), AB₂O₄ type- Spinel structure, Normal & Inverse, Factors causing distortion in spinel, A₂B₂O₇ type: Pyrochlores (La₂Sn₂O₇).

Unit-II: Imperfections in Materials

Perfect &Imperfect crystals, point defects, Interstitial, Schottky defect, Frenkel defect, line defect & other entities, thermodynamics of Schottky& Frankel defects, Dissociation, theory of dislocation, plane defects-Lineage boundary, grain boundary, stacking fault, 3D defects, Defects & their concentrations, ionic conductivity in solids, Non stoichiometric compounds. Electronic properties of Non-stoichiometric oxides, solid electrolytes, pyknometric & electrical conductivity methods of study of defects, photo-radiation effects on solid nature and properties, photography, colour centers, order-disorder changes, defects, imperfection equilibrium, atom movements, and defect interactions.

Unit III: Synthesis and Characterization of Nanomaterials

General introduction to Nanomaterials, Nanoscience and nanotechnology, History, Chemical Methods: Metal nanoparticles: Reduction method, Semiconducting or composite nanomaterials: Hydrothermal and Solvothermal method, Sol-gel, Arrested Precipitation, and other methods include) Langmuir-Blodgett, Micelles-Microemulsions. Characterization Tools: Electron Microscopy (TEM & SEM), Probe Microscopy (STM & AFM), Diffraction Technique (XRD), UV-Visible-NIR spectroscopy, BET.

Unit IV: Properties and Applications of Nanomaterials 15 hrs.

Properties of Nanomaterials: Optical, Magnetic, Electrical, Mechanical, Structural properties Illustrative Nanomaterials: Carbon nanostructures (CNTs, Graphene and its derivatives, fullerenes, Metal oxides (TiO2 and ZnO) & its composites, Quantum dots, Core-Shell nanoparticles, Different morphological nanomaterials. Applications in the various fields: Electronic devices, Energy generation and storage, Automobiles, Sports and toys, Textile Industries, Cosmetics Products, Domestic appliances, Sensors, Biotechnology and medical field, Space and Defense, Catalysis, Environment.

Reference Books:

- New Directions in Solid State Chemistry (Second Eds.), C.N.R.Rao and G. Gopalkrishnan, Cambridge Oxford Press.
- 2. A basic course in crystallography, JAK Tareen, TRN Kutty, Universities press.
- 3. Essentials of crystallography, M.A. Wahab, Narosa Publications.
- 4. Synthesis of Inorgnic Materials: Ulrich Schubert, Nicola Hüsing.
- 5. Solid State Chemistry: Lasley E. Smart, Elaine A. Moore.
- 6. Introduction to Solid State Physics: Charles Kittel.
- 7. Solid State Chemistry: A. H. Hanny
- 8. Wilcox: Preparation and Properties of Solid State Materials: Vol I & II, Dekker
- 9. Hagenmuller, Preparative Methods in Solis State Chemistry
- 10. Lohn Wulff, The Structure and Properties of Materials Vol. IV, Electronic Properties (Wily Eastern)
- 11. Chemistry of Imprefect Crystals (Holland) E.A. Kroger
- 12. Solid State Chemistry A. R. West,
- 13. Principles of the Solid-State Chemistry, Wiley Eastern. H. V. Keer:

Course Outcome (COs):

CO1: At the end of the course students should be able to explain the bonding and structures of the solid-state materials.

CO2: After completion of this course students will be able to explain the various defects present in the solid-state materials and their impact on electronic and structural properties of the same.CO3: Students will be able to explain the various synthesis methods and advanced instrumentation tools used for characterization of nano-materials.

CO4: At the end students will be able to explain the optical, magnetic and structural properties of the nanomaterials and will be able to explain their applications in various industrial fields such as electronic devices, Energy generation and storage, Automobiles, Sports and toys, Textile Industries, Cosmetics Production, etc.

RP-ICH405 Research Project

(6 Cr, 180 Hrs) 150 Marks

See Annexture-I for details.

Note: Study tour is the part of your syllabus for M.Sc. Part- II. Students shall visit Chemical Industries in India.

Name of Program: M.Sc. Organic Chemistry

M. Sc. Organic Chemistry, a post-graduate degree program of the Shivaji University, is one of the best in the country because it's curriculum involves most advanced topics like Organic reaction mechanism, Advance spectroscopic methods, Advance synthetic methods, Drug and Heterocycles, Theoretical Organic Chemistry, Stereochemistry, Chemistry of Natural Products, Applied organic chemistry, etc. and the practical training based on these advanced topics required to understand problems of the present time. Successful students of this course are capable of doing independent research work not only in relevant world class laboratories but also in R&D sectors and in quality teaching institutes.

1. Program Outcomes (POs)

Program Outcomes (POs)

- PO1. Students will be able to acquire in depth knowledge about fundamental as well as applied organic chemistry concepts.
- PO2. Students will be able to solve various problems by identifying the essential parts of a problem, formulate strategy for solving the problem, applying appropriate techniques to arrive at a solution, test the precision an accuracy of the solution and interpret the results.
- PO3. Students will be able to acquire domain specific knowledge and technical skills needed for employment in industries, teaching fields and pursue research.
- PO4. Students will be able to apply the fundamental knowledge to address the cross-cutting issues such as sustainable development.
- PO5. Students will get perfect insight into organic chemistry research ethics for production of quality research.
- PO6. Students will be able to communicate effectively i. e. being able to comprehend and write effective reports, make effective presentations and documentation and capable of expressing the subject through technical writing as well as through oral presentation.

2. Program Specific Outcomes (PSOs)

- PSO 1. Students will be able to qualify competitive examinations like NET, SET, GATE, etc.
- PSO 2. Students will have opportunities to serve in different Chemical, Pharmaceutical as well as food and agrochemical industries.
- PSO 3. Students will have global level research opportunities in Ph.D. programme.

- PSO 4. Collaborate effectively on team-oriented projects in the field of Chemistry or other related fields.
- PSO 5. Students can start their own chemical industry / business (entrepreneurship).
- PSO 6. Students will be able to interpret NMR, MS, IR for structural elucidation.

3. Framework of NEP 2.0 as per NEP-2020 for M. Sc. Degree in Organic Chemistry

Year Level Sem		Major	RM	OJT/FP	RP	Cumm.	Degree
	Mandatory	Elective [Chose any one elective]				Cr.	
I 6.0 I	OCH101 (4 Cr)	E-ICH103 (4 Cr) OR	RM-CH106			22	PG Diploma in
	ICH102 (4 Cr)	E-OCH103 (4 Cr) OR	(4 Cr)				Organic Chemistry
	PRCH104 (4 Cr-Major	E-PCH103 (4 Cr) OR					(After 3yr B.Sc.
	Experiments- 5 from	E-ACH103 (4 Cr) OR					Degree)
	each Section)						Note: Common
	PRCH105 (2 Cr-Minor						practicals for M.Sc
	Experiments-3 from						I
	each Section)						
_				0/1-		22	M.ScII will be
Ш	PCH201 (4 Cr)	E-ICH203 (4 Cr) OR		OCH206			discipline specific
	ACH202 (4 Cr)	E-OCH203 (4 CF) OK		(4 Cr) UK			i.e. Organic
	PRCH204 (4 Cr-Major	E-PCH203 (4 Cr) OR		PP-			Chemistry oriented
	Experiments-) from	E-ACH203 (4 Cr)		OCH206 (4			
	each Section)			[Ann One]			
	PRCH205 (2 Cr Minor			[Any One]			
	Experiments-5 from each						
Cum Cr. for PG Dinlows	38 (1011))	e	4	4		44	
Cuill: CI: IOI I O Dipiolila	Exito	ntion: PG Diploma (40-44 Credits) a	fter Three Year U	JG Degree			
II 6.5 III	OCH301 (4 Cr)	E-ICH304 (4 Cr) OR			RP-	22	PG Degree After 3-
	OCH302 (4 Cr)	E-OCH304 (4 Cr) OR			OCH306		VrUG
	OCH303 (4 Cr)	E-PCH304 (4 Cr) OR			(4 Cr)		Or
	PR-OCH305 (2 Cr)	E-ACH304 (4 Cr) OR					PG Degree after 4-
							YrUG
IV	OCH401 (4 Cr)	E-ICH404 (4 Cr) OR			RP-	22	Note: All the
	OCH402 (4 Cr)	E-OCH404 (4 Cr) OR			OCH405		practicals/Project
	OCH403 (4 Cr)	E-PCH404 (4 Cr) OR			(6 Cr)		will be discipline
		E-ACH404 (4 Cr) OR					specific i.e. Organic
							Chemistry oriented
Cum. Cr. For 1 Year PG	28	8	4	4	10	44	
Degree					14		
Cum. Cr. For 2 Year PG	54	16	4	4	10	88	

M.Sc. Organic Chemistry

4. Course Structure: M.Sc. Part-II, Organic Chemistry

Semester III

Major Mandatory

Course Code	Course Title	Credits
OCH301	Organic Reaction Mechanism	4
OCH302	Advanced Spectroscopic methods	4
OCH303	Advanced Synthetic methods	4
PR-OCH305	Practical Course	2
RP-OCH306	Research Project	4

Major Elective (Choose any one)

Course Code	Course Title	Credits
E-ICH304	Organometallic and Bioinorganic	4
	Chemistry	
E-OCH304	Drug and Heterocycles	4
E-PCH304	Solid State Chemistry	4
E-ACH304	Environmental Chemical Analysis	4
	and Control	

Semester IV

Major Mandatory

Course Code	Course Title	Credits
OCH401	Theoretical Organic Chemistry	4
OCH402	Stereochemistry	4
OCH403	Chemistry of Natural Products	4
RP-OCH405	Research Project	6

Major Elective (Choose any one)

Course Code	Course Title	Credits
E-ICH404	Energy and Environmental	4
	Chemistry	
E-OCH404	Applied Organic Chemistry	4
E-PCH404	Surface Chemistry	4
E-ACH404	Applied Analytical Chemistry	4

5. Detailed Syllabus

M. Sc. II (Sem III) Organic Chemistry

OCH 301: Organic Reaction Mechanism

UNIT-I: Methods of determining reaction mechanism

(A) Kinetic Methods: Order and Molecularity, Methods of following reaction rates, Types of reactions: 1st, 2^{nd,} and 3rd order reactions, Reversible, Consecutive, and Parallel reactions. Energy of Activation, Entropy of Activation, Effect of Ionic strength, Solvent effect, and Kinetic isotopic effect

(B) Non-Kinetic Methods: Identification of reaction products, Testing of the possible

intermediates, Trapping of the intermediates, Isotopic labeling, Reaction catalysis, Crossover experiments, Stereochemical studies, and Use of physical properties. Hammett and Taft equations.

UNIT-II: Pericyclic reactions

Molecular orbital symmetry, Frontier orbital of ethylene, 1,3- butadiene, 1,3,5-hexatriene and allyl system, Classification of peri cyclic reaction, Wood-ward Hoffman correlation diagrams, FMO and PMO approach, Electrocyclic reactions, Conrotatory and disrotatary motions, 4n, 4n+2 and allyl systems, Cycloaddition, and supra and antara facial additions, 4n and 4n+2 systems, 2+2 additions of ketenes, 1,3-dipolar cycloaddition and Chelotropic reactions, Sigmatropic rearrangement, supra and antarafacial shifts of H, Sigmatropic shifts involving carbon moieties, (3,3) and (5,5) sigmatropic rearrangement and Claisen and Cope and Aza Cope rearrangement, Ene reaction.

UNIT-III: Study of the intermediate and name reactions

- (A) Ylids: Nitrogen, Sulfur and Phosphorous ylides: Synthesis and applications in organic synthesis.
- (**B**) Name Reactions: Alkyne metathesis reaction, Weinreb ketone synthesis, Petasis reaction, Henry reaction, Corey Kim oxidation. Reactions of carboxylic acids and esters.

UNIT-IV: Free radical reactions

Types of free radical reactions, Detection by ESR, Mechanism of free radical substitution, Neighboring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in attacking radicals. The effect of solvent on reactivity. Allylic halogenation (NBS), Oxidation of aldehydes to carboxylic acids, Auto-oxidation, Coupling of alkynes, Arylation of aromatic compounds by diazonium salt, Sandmeyers reaction, Hunsdiecker reaction.

Reference Books:

- 1. A guide book to mechanism in organic chemistry (orient- Longmans)- Peter Sykes
- 2. Organic Reaction Mechanism (Benjumin)- R. Breslow
- 3. Mechanism and structure in Organic Chemistry (Holt Reinhartwinston)- B. S. Gould
- 4. Organic chemistry (McGraw Hill)- Hendrikson, cram and Hammond
- 5. Basic principles of organic chemistry (Benjamin) J. D. Roberts and M. C. Caeserio.

15 hrs.

15 hrs.

- 6. Reactive intermediates in organic chemistry, (J. Wiley) N. S. Issacs.
- 7. Organic reaction mechanism (McGraw Hill) R. K. Bansal
- 8. Fundamentals of photochemistry K. K. Rohtagi- Mukherji Wiley- Eastern
- 9. Essentials of molecular photochemistry, A. Gilbert and J. Baggott. Blackwell Scientific Publication.
- 10. Molecular photochemistry, N.J. Urro, W. A. Benjamin
- 11. Introductory photochemistry. Cox and T. Camp McGraw -Hill
- 12. Photochemistry R.P. Kundall and A. Gilbert. Thomson Nelson.
- Strategic applications of named reactions in organic synthesis by Laszlo Kurti and Barbara Czako.
- 14. Organic photochemistry J. Coxon and B. Hallon Cambridge University press.

Course Outcomes (COs):

CO No. On completion of the course, students will be able to:

- CO1 Adopt the knowledge about the pathway and determine reaction rates using kinetic and non-kinetic methods. This involves steps such as reaction rate determination, order and molecularity, testing and trapping of intermediates, stereochemistry, and the Hammet-Taft equation.
- CO2 Familiarize with the concept of Pericyclic reactions, Woodward-Hoffmann correlation diagrams, and the Frontier Molecular Orbital (FMO) and Molecular Orbital (PMO) approaches. Understand conrotatory and disrotatory motion, and be able to identify reactions as 4n, 4n+2, and 2+2 addition of ketenes. Additionally, learn about sigmatropic shifts (3,3) and (5,5), Claisen and Cope rearrangements, and Aza-Cope rearrangement.
- CO3 Learn about the mechanisms, stereochemistry, migratory aptitude, and applications of different name reactions such as Dienone-phenol, Favorskii, Smiles, Brooke, Neber, Stevens, and Sommelet-Houser rearrangement reactions.
- CO4 Adapt the knowledge about photochemistry photochemical reactions, their types, and laws of photochemistry. Also, know quenching and chemiluminescence.

OCH 302: Advanced Spectroscopic methods

UNIT-I: Study of Ultraviolet and IR Spectroscopy

(A) Ultraviolet Spectroscopy:

Woodward-Fisher rules for conjugated dienes and carbonyl compounds, Calculation of λ max of conjugated dienes and carbonyl compounds. Ultraviolet spectra of aromatic and heterocyclic compounds, Steric effect in biphenyls.

(B) IR Spectroscopy:

Characteristic vibrational frequencies of (i) alkanes, (ii) alkenes, (iii) alkynes, (iv) aromatic compounds, (v) alcohols, (vi) ethers, (vii) phenols, (viii) amines. Detailed study of vibrational frequencies of carbonyl compounds; (i) ketones, (ii) aldehydes (iii) esters (iv) amides (v) acids (vi) anhydrides (vii) lactones (viii) lactams, and (ix) conjugated carbonyl compounds. Effect of hydrogen bonding and solvent effect on vibrational frequencies, Overtones, combination bands, and Fermi resonance, FT-IR of gaseous; solids and polymeric materials.

UNIT-II: NMR Spectroscopy

General introduction and definition; chemical shift, spin-spin interaction, shielding mechanism of measurement, Chemical shift values, and correlation for protons bonded to (a) carbons: aliphatic, olefinic, aldehydic, and aromatic and (b) other nuclei: alcohols, phenols, enols, acids, amines, amides and mercaptons, Chemical exchange; effect of deuteration, Complex spin-spin interaction (first order spectra) between (i) two (ii) three (iv) four and (v) five nuclei, Virtual coupling, Stereochemistry; hindered rotation, Karplus curve variation of coupling constant with dihedral angle, Simplification: Simplification of complex spectra, nuclear magnetic double resonance, shift reagent, solvent effect. Fourier transform technique, Nuclear overhauser effect [NOE], NMR of F, and P nuclei.

UNIT-III: Mass Spectrometry

Introduction of MS, Ionization methods; (i) EI, (ii) CI, (iii) FD (iv) FAB, and (v) MALDI-TOF, Factors affecting on fragmentation, Ion analysis, Ion abundance. Molecular ion peak, Metastable peak, McLafferty rearrangement, Nitrogen rule. Mass spectral fragmentation of organic compounds; (i) hydrocarbons (aliphatic and aromatic), (ii), carbonyls (aldehydes, ketones, acids, acid chlorides, esters, amides), (iii) halogen compounds (iv) amines, (iv) nitro compounds, Highresolution mass spectrometry (HRMS).

15 hrs.

15 hrs.

(5)

(10)

UNIT-IV: Study of ¹³C NMR and Combined problems

(A) Carbon-13 NMR Spectroscopy:

General considerations; chemical shift; aliphatic, olefinic, alkyne, aromatic, heteroaromatic, and carbonyl compounds, problems associated with ¹³C, FT- NMR, proton decoupled off-resonance.

(B) Structural Problems:

(8)

(7)

15 hrs.

Structural problems based on combined spectroscopic techniques (including reaction sequences)

Reference Books:

- 1. V.M. Parikh, Application spectroscopy of organic molecules. (Mehta)
- 2. D.W. Williams and Flemming, Spectroscopic methods of organic compound.
- 3. Silverstein and Basslar, Spectroscopic identification of organic compounds V.M. Parikh ORPTION SPECTROSCOPY OF ORGANIC MOLECULES (J. Wiley)
- 4. P.S. Kalsi Spectroscope of organic compounds (New age publisher)
- 5. J.R. Dyer. Application of absorption spectroscopy of organic compounds.
- 6. Jackman and Sterneil, Application of NMR spectroscopy
- 7. Nuclear magnetic resonance. J.D. Roberts (J. Wiley)
- 8. Theory and application of U.V. Jafee and Orchin.
- 9. Mass spectroscopy K. Benjamin.
- 10. The mass spectra of organic molecules. Beynon J H.
- 11. Interpretation of carbon 13 NMR Wehli F.W, Marchand A. P. (J. Wiley)
- 12. Organic Spectroscopy W. Kemp, ELBS
- 13. Instrumental methods of analysis CBS. Willard Merritt and Dean.
- 14. Mass Spectroscopy. Das and Jame
- Organic structural spectroscopy: J. B. Lambert, S. Gronert, H. F. Shurvell, D. Lightneli, R. G. Cooks (Prentice Hall 2nd edition).

Course Outcomes (COs):

CO No. On completion of the course, students will be able to:

- CO1 Learn about the principles and theory behind UV and IR spectroscopy, including molecular vibrations due to IR radiation absorption and electronic excitations from UV radiation absorption. This will help students identify unknown organic compound structures and recognize functional groups such as alcohol, aldehyde, ketone, ester, and aromatic compounds. They will also study overtones, combination bands, and Fermi resonance in FT-IR spectroscopy.
- CO2 Recap proton NMR spectroscopy, factors affecting coupling constants, analyze first-order spectra, simplify complex spectra, understand second-order spectra, effect of deuteration, and spectra of Homotopic, Enantiotopic, and Diastereotopic systems. Also, learn about the Advanced NMR technique, Fourier transform technique, Nuclear Overhauser Effect (NOE), COSEY, NOSEY, and resonance of F19 and P31 nuclei.
- CO3 Learn about ion production methods (EI, CI, FD, and FAB) and factors affecting fragmentation analysis. Also understand mass spectral fragmentation of functional groups (e.g., aldehydes, ketones, esters, alcohols) to solve mass spectroscopy problems.
- CO4 Understand the concept of C13 NMR spectroscopy chemical shift values of alkanes, alkenes, alkynes, aromatic compounds, carbonyl and heterocyclic compounds. Also learn this advanced C13 technique NOE, DEPT, HETCOR and heteronuclear coupling. They will become confident to solve the problems on C13 NMR.

OCH 303: Advanced Synthetic methods

UNIT-I: Disconnection Approach

- (a) Terms involved in retrosynthesis; synthons, synthetic equivalents, disconnection approach, functional group interconversions.
- (b) Importance of the order of events in organic synthesis
- (c) Chemoselectivity, Regioselectivity, and Stereoselectivity, Protecting groups,
- (d) One group C-X and two group disconnections in (i) 1, 2, (ii) 1, 3 (iii) 1, 4, and (iv) 1, 5-difunctional compounds,
- (e) Retrosynthesis of (i) alkanes (ii) alkene, (iii) acetylenes, (iv) nitro (v) alcohols (vi) carbonyl compounds, (vii) amines, (viii) aromatic heterocycles (ix) 3, 4, 5 and 6 membered rings.
- (f) Reversal of polarity (Umpolung).
- (g) Use of Diels-Alder reaction, Michael addition, and Robinson annulation in retrosynthesis.

UNIT-II: Applications of the following in organic synthesis 15 hrs.

- (A) Reagents: Lithium diisopropylamide(LDA) Dicyclohexyl carbodiimide(DCC), lead tetra acetate, PPA, Diazomethane, ozone, phase transfer catalyst, Selenium dioxide, Dess-Martin periodinane, and iodoisobenzyldiacetate, periodic acid
- (**B**) **Reactions:** Woodward-Prevost hydroxylation, Barton and Shapiro reaction, Hoffmann– Loffler-Fretag, Peterson synthesis, Olefin metathesis using Grub's catalysts.

UNIT-III: Applications of metals and ligands in organic synthesis	15 hrs.
(A) Applications of metals in organic synthesis	
(i) Ti, (ii) Ce, (iii) Tl and (iv) Si	
(B) Applications of ligands in organic synthesis: Synthesis and Applications	
(i) Phosphines, (ii) N-heterocyclic carbenes (NHC), and (iii) Oxazoline	
UNIT-IV: Applications of the following methods in organic synthesis	15 hrs.
(a) Synthesis and applications of Merrifield resin	
(b) Electro-organic synthesis	
(c) Enzyme catalyzed reaction	
(d) Solvent free synthesis	
(e) Multicomponent reactions	

- (f) Microwave techniques and their applications
- (g) Ultrasound techniques and their applications
- (h) Mechanochemical synthesis

Reference Books:

- 1. Designing of organic synthesis. S. Warren
- 2. Organic synthesis J. Fuhrhop & G. Penzlin. (2nd ed.)
- 3. Some modern methods of organic synthesis.Carruthres:
- 4. Modern synthetic reaction. H. O. House
- 5. Reagent in organic synthesis. Fieser & Fieser
- 6. Principle of organic synthesis. R. O. C. Norman
- 7. Advanced organic Chemistry. Carey & Sundharg
- 8. Organic synthesis. P. E. Realand:
- 9. Comprehensive organic Chemistry. Bartan and Ollis :
- 10. Organic reactions. R. Admas:
- 11. Advances in organometallic Chemistry. Stone & West:
- 12. Transition metal intermediate in organic synthesis. C. W. Bird:
- 13. Organometallic in organic synthesis. Swan & black :
- 14. Synthesis of prostaglandins. A. Mitra :
- 15. Total synthesis of natural products. John Apsimon:
- Phosphorus ligands in homogeneous catalysis: Design and synthesis by Paul C. J. Kamer.
- Phosphorus ligands effect in homogeneous catalysis and rational catalyst design by Jason A. Gillespie and Erik Zuidema. Polymers as aid in organic synthesis. M. K. Mathur, C. K. Narang & R. E. Williams:
- 18. Polymer supported reaction in organic synthesis. P. Hodge & D. C. Sherrington:
- 19. Enzyme catalysed reactions.C. J. Gray:
- 20. Electroorganic Chemistry. T. Shona:
- 21. Phase transfer catalyst in organic synthesis. Weber & Gokel

Course Outcomes (COs):

CO No. On completion of the course, students will be able to:

- CO1 Understand the concept of the disconnection approach through the introduction of synthons, synthetic equivalents, and functional group interconversions. Also, understand retrosynthesis of difunctional compounds. Importance of the order of reaction in organic synthesis. They will learn Diel's Alder reaction, Michael addition, Robinson annulation, and what is meant by Umpolung reaction.
- CO2 Study the applications of different reagents in chemical reactions and also study of Woodward – Prevost hydroxylation, Barton and Shapiro reaction as well as Grub's catalysis.
- CO3 Learn how the different metals and ligands in organic chemistry.
- CO4 Learn the new concept of supramolecular chemistry, advanced synthetic methods by using microwave ovens, ultrasound waves, using enzymes, electroorganic synthesis, use of multicomponent reactions as well as the use of Ionic liquids in chemical reactions.

PR-OCH305 Organic Chemistry Practicals (2 Cr.) 60 hrs.

A) Qualitative Analysis

Separation, purification and identification of compounds (any two) of ternary mixtures using **semi-microanalysis**, TLC, column chromatography and chemical tests. IR spectra to be used for functional group identification.

B) Quantitative analysis

1. Two step Preparations (Any Five)

- a) Preparation of m-Nitroaniline
- **b**) Preparation of Benzanilide from benzophenone
- c) Preparation of Phthalimide
- d) Preparation of N-Bromosuccinimide
- e) Preparation of 4-methyl -7-acetoxy coumarin
- f) Preparation of 1, 2, 3, 4- Tetrahydro carbazole
- g) Preparation of p-ethoxy acetanilide

Reference books:

- 1. Textbook of Practical Organic Chemistry A. I. Vogel.
- 2. Practical Organic Chemistry Mann & Saunders.
- 3. A Handbook of Quantitative & Qualitative Analysis- H. T. Clarke.
- 4. Organic Synthesis Collective Volumes by Blat

NOTE: Student should perform their practical work in the laboratory minimum 15 days in one semester for 2 credits.

RP-OCH306 Research Project (4 Cr)

See Annexture-I for details.

M. Sc. II (Sem IV) Organic Chemistry

OCH 401: Theoretical Organic Chemistry

UNIT-I: Molecular Orbital Theory

Aromaticity in benzenoids, alternant and non-alternant hydrocarbon, Huckels rule, energy level of π - molecular orbital and concept of aromaticity, calculation of energies of orbitals cyclic and acyclic systems. Determination energies and stabilities of different systems calculation of charge densities PMO theory and reactivity index.

UNIT-II: Non benzenoid aromatic Compounds

Aromaticity in non-benezenoid compounds Annulenes and heteroannulenes, fullerenes, azulene, fulvene, tropylium salts, ferrocene, five-membered systems. Crown ether complexes, cyclodextrins, cryptands, catenanes, and rotaxanes, bonding in fullerenes.

UNIT-III: Green Chemistry

Introduction to the principles of green chemistry – prevention of waste, atom economy, less hazardous chemical syntheses, designing safer chemicals, safer solvents and auxiliaries, design for energy efficiency, reducing derivatives, renewable feedstock, catalysis, design for degradation, real-time analysis for pollution prevention, and inherently safer chemistry for accident prevention. Green synthesis, clean routes using supercritical solvents, ionic liquids, and water.

UNIT-IV:

A) Kinetic and thermodynamic control of reactions

15 hrs.

15 hrs.

15 hrs.

15 hrs.

(9)

Nitration and Sulphonation of naphthalene, Wittig, Enolization, Friedel-Crafts and Diels Alder reactions.

(6)

B) Non-classical carbocations: Formation, stability, and reactivity.

Reference Books:

- 1. Lehar and Merchand: Orbital Symmetry.
- 2. R. B. Woodward and Hoffman: Conservation of orbital symmetry.
- 3. P. T. Anastas, J. C. Werner: Green Chemistry: Theory and Practice
- 4. V. K. Ahluwalia: Green chemistry, A textbook
- 5. V. K. Ahluwalia, R. S. Verma: Green Solvents: For Organic Synthesis
- 6. Ginsburg: Nonbenzenoid aromatic compound.
- 7. A. Streitwieser: Molecular orbital theory for organic chemistry.
- 8. E. Cler: The aromatic sextet.
- 9. Lloyd: Carbocyclic non- benzenoid aromatic compounds.
- 10. W. B. Smith: Molecular orbital methods in organic chemistry.
- 11. Grratt; Aromaticity

Course Outcomes (COs):

CO No. On completion of the course, students will be able to:

- CO1 Understand the concept of aromaticity, Huckel's rule, the energy level of pimolecular orbital, calculation of energies of cyclic and acyclic systems, calculation of charge densities, PMO theory, and reactivity index.
- CO2 Learn synthesis and reactions of Linear and Non-linear polynuclear hydrocarbons.
 Understand the concept of aromaticity and anti-aromaticity as well as the concept of
 3- and 5- 5-membered carbocyclic compounds, crown ethers, cyclodextrins, catenanes, and rotaxanes.
- CO3 Understand the types of free radicals, detection by ESR, reaction mechanism, and reactivity. They also learn the effect of solvent on reactivity, Sandmeyer's reaction, Hunsdiecker reaction.
- CO4 Learn about the Kinetic and thermodynamic control of nitration and sulphonation, about Wittig reaction, Enolization, F. C. reaction, and Diel's Alder reaction. Understand Non-classical carbonation - Formation, stability, reactivity, and synthetic applications.

OCH 402: Stereochemistry

l5 hrs.
(4)
1,
(4)
and
enthol,
(7)

UNIT- II: Conformational analysis and reactivity of the fused and bridged ring system 15 hrs.

- A) Fused rings: Types of fused ring systems; (i) Fused bicycles: cis and trans-decalins, octalins, decalols, (ii) Fused poly-bicycles: perhydroanthracene and perhydrophenanthrene (iii) effect of angular methyl group on conformation of fused ring system.
- **B) Bridged rings:** Types of bridged ring systems, nomenclature, bridged bicycles: heptanes and octane, stereochemical restrictions, Bredt's rule.

UNIT- III: Stereoselective Synthesis	15 hrs.
A) Stereoselective addition of nucleophiles to carbonyl group	(6)

Cram's rule, Felkin Ahn rule, Houk's model, Cram's chelate model. Asymmetric synthesis by use of chiral auxiliaries, use of chiral substrates, reagents, and catalysts

B) Asymmetric Synthesis

Asymmetric epoxidation of allylic alcohols (Sharpless Epoxidation), Dihydroxylation of olefins: Sharpless asymmetric dihydroxylation, Upjohn process, Milas hydroxylation.

(9)

Asymmetric Diels-Alder Reactions using chiral Lewis acids: Chiral bissulfonamides (Corey's catalyst).

UNIT- IV: Stereochemistry of compounds containing no chiral carbon atoms	
A) Stereochemistry of allens, sprains and biphenyls, assignment of configuration	
B) Configuration of diastereomers	
Geometrical isomerism based on physical and chemical methods.	
C) O.R.D. and C.D.	(7)

ORD and CD curves with Cotton effect. Empirical and semi-empirical rules; The octant rule, helicity rule, Lowe's rule, and axial haloketone rule.

Reference Books:

- 1. E.L. Eliel: Stereochemistry of carbon compounds.
- 2. D. Nasipuri : Stereochemistry of organic compounds
- 3. P.S. Kalsi: Stereochemistry, Conformation and Mechanism.
- 4. Eliel, Allinger, Angyal and Morrison: Conformational analysis.
- 5. Hallas: Organic stereochemistry
- 6. Mislow and Benjamin: Introduction to Stereochemistry.
- 7. H. Kagan: Organic stereochemistry.
- 8. Carl Djerassi; Optical Rotatory Dispersion.
- 9. P. Crabbe: Optical Rotatory Dispersion and C.D.

Course Outcomes (COs):

CO No. On completion of the course, students will be able to:

- CO1 Approve the knowledge of about stereoselective, stereospecific synthesis, chemoselective and regioselective reactions. Undestand the enantioselective synthesis, reactions with hydride donar, catalytic hydrogenation via chiral hydrazones and oxazolines etc.
- CO2 Understand in depth stability and reactivity of diastereoisomers, Curtin-Hammett principle, some aspects of stereochemistry of ring compounds. The shapes of the 5, 6 and 7 membered rings. Also, they will learn the conformational effects in medium sized rings and the concept of I-strain.
- CO3 Knowledge about conformation and configuration of fused bicyclic rings and
bridged rings, stereochemical restrictions, and Bredt's rule.

Understand O. R. D. and C. D. curves, circular dichroism, the Octane rule and axial haloketone rule.

CO4 Explain the stereochemistry of Allenes, Spiranes, and Biphenyls and how to assign the configuration and by using physical and chemical methods.

OCH 403: Chemistry of Natural Products

UNIT-I: Terpenoids

Introduction of natural products and Terpenoids: Introduction of natural products: Classification and isolation methods. Terpenoids: Structure and synthesis of camphor, carvone, abietic acid, zingiberene, α -santonin, β -cuparenone. Biogenesis of abietic acid.

UNIT-II: Alkaloids

Structure, stereochemistry, synthesis, and biosynthesis of the following: Morphine, Reserpine, Papaverine, and Lysergic acid. Biogenesis of Coniine.

UNIT-III: Steroids

Occurrence, nomenclature, basic skeleton, Diels hydrocarbon. Study of the following: ormones (Structure and synthesis): Cholesterol, Androsterone, Testosterone, Estrone, Progesterone, Aldosterone and cortisone Bile acid (only synthesis) and biosynthesis of lanosterol.

UNIT-IV: Study of Prostaglandins, Lipids and Vitamins	15 hrs.
A) Prostaglandins:	(5)
Occurrence, nomenclature, classification, biogenesis and physiological effects, Synt	hesis of
PGE2 and PGF2.	
B) Lipids:	(4)
Classification, Role of Lipids, Fatty acids and glycerol derived from oils and fats.	
C) Vitamins:	(6)
Synthesis and structure of biotin, vitamin B1 and B2, Biological functions of Vitam	in B ₆ , D
and E.	

Reference Books:

- 1. Apsimon: The total synthesis of natural products.
- 2. Manskey and Holmes: Alkaloids

15 hrs.

15 hrs.

- 3. A.A. Newmen: Chemistry of Terpenes.
- 4. P. D B. Mayo: The chemistry of natural products.
- 5. Simonson: Terpenes.
- 6. T.W. Goddwin: Aspects of terpenoid chemistry and biochemistry.
- 7. R.T. Slicken staff A.C. Ghosh and G.C. Wole: Total synthesis of steroids.
- 8. The chemistry of natural products, vol. Nakanishi
- Biochemistry of Lipids, Lipoproteins and membranes by Neele Ridgway and Roger McLeod
- 10. Membranes (New comprehensive biochemistry) by J E Vance and E Vance
- 11. Schaum's easy outline of biochemistry by Philip W Kuchel.

Course Outcomes (COs):

CO No. On completion of the course, students will be able to:

- CO1 Learn the classification, isolation of terpenoids, structure, and synthesis of Camphor, Carvone, Abietic acid, zingiberene, alpha-santonin, and beta-caryophyllene.
- CO2 Know all about Alkaloids the occurrence, isolation, structures, functions, stereochemistry, and synthesis of Morphine, Reserpine, Atropine, and Conin alkaloids.
- CO3 Learn the occurrence, nomenclature, and basic skeleton of steroids as well as the synthesis of hormones like cholesterol, Androsterone, Testosterone, and Estrone. Also study the nomenclature, classification, biogenesis, physiological effects, and synthesis of prostaglandin PGE2 and PGF2.
- CO4 Study about the Vitamins as well as synthesis and biological functions of vitaminsB1, B2, B5, B6, and Biotin i.e. vitamin H.

RP-OCH405 Research Project (6 Cr)

See Annexture-I for details.

Note: Study tour is the part of your syllabus for M.Sc. Part- II. Students shall visit Chemical Industries in India.

Name of Program: M.Sc. Physical Chemistry

M. Sc. Physical Chemistry, a post-graduate degree program of the Shivaji University, is one of the best in the country because it's curriculum involves most advanced topics like *ab initio* methods, semiempirical methods, density functional theory, molecular simulations, molecular dynamics, statistical mechanics of quantum particles, irreversible thermodynamics, molecular spectroscopy, nanomaterials, electrochemistry at interfaces, etc. and the practical training based on these advanced topics required to understand problems of the present time. Successful students of this course are capable of doing independent research work not only in relevant world class laboratories but also in R&D sectors and in quality teaching institutes.

1. Program Outcomes (POs)

- PO1: Understanding fundamental principles and laws of physical chemistry
- PO2: Development of abilities to study and understand properties of materials
- PO3: Design and testing of electrochemical cells and electrochemical properties of materials
- PO4: Understanding forces responsible for various types of structure property correlations
- PO5: Studies of physicochemical properties of novel materials including nanomaterials
- PO6: Studies of protein-ligand binding interactions.
- PO7: Solid material design, property measurements, structural analysis and application testing
- PO8: Empowering the students to do independent research of high caliber.

2. Program Specific Outcomes (PSOs)

- PSO1: Electronic structure calculation and property analysis or prediction
- PSO2: Understanding kinetics and dynamics of materials in gas and condensed phases
- PSO3: Structure elucidation and estimation of molecular properties

PSO4: Independently perform a computer simulation to predict structures, reaction paths, molecular/material properties, etc.

3. Framework of NEP 2.0 as per NEP-2020 for M. Sc. Degree in Physical Chemistry

Class	SEM	Level	Mandatory Subject	Elective Choose any One	RM (4 Cr)	OJT/FP (4 Cr)	RP	Cumm. Cr	Degree
M.Sc. II	III	6.5	PCH.301 (4Cr)	E-ICH.304 (4Cr) OR			RP-PCH.	22	M.Sc. Degree
			PCH.302 (4Cr)	E-OCH.304 (4Cr) OR			306 (4 Cr)		in Physical
			PCH.303 (4Cr)	E-PCH.304 (4Cr) OR E-ACH.304 (4Cr) OR					after 3/4 yr.
			PR-PCH305 (2 Cr)						UG
	IV	6.5	PCH.401 (4Cr)	E-ICH.404 (4Cr) OR			RP-PCH	22	
			PCH.402 (4Cr)	E-OCH.404 (4Cr) OR F-PCH 404 (4Cr) OR			405 (6 Cr)		
			PCH.403 (4Cr)	E-ACH.404 (4Cr) OR					
Cum. Cr. I	For 1 Yo Degree	ear PG	26 Cr	8 Cr			10	44	

5. Course Structure: M.Sc. Part-II, Physical Chemistry

Semester III

Major Mandatory

Course Code	Course Title	Credits
PCH301	Advanced Quantum Chemistry	4
PCH302	Electrochemistry	4
PCH303	Molecular Structure-I	4
PR-PCH305	Physical Chemistry Practical-V	2
RP-PCH306	Research Project	4

Major Elective (Choose any one)

Course Code	Course Title	Credits
E-ICH304	Organometallic and Bioinorganic	4
	Chemistry	
E-OCH304	Drug and Heterocycles	4
E-PCH304	Solid State Chemistry	4
	-	
E-ACH304	Environmental Chemical Analysis	4
	and Control	

Semester IV

Major Mandatory

Course Code	Course Title	Credits
PCH401	Thermodynamics and Molecular Modelling	4
PCH402	Chemical Kinetics	4
PCH403	Molecular Structure-II	4
RP-PCH405	Research Project	6

Major Elective (Choose any one)

Course Code	Course Title	Credits
E-ICH404	Energy and Environmental Chemistry	4
E-OCH404	Applied Organic Chemistry	4
E-PCH404	Surface Chemistry	4
E-ACH404	Applied Analytical Chemistry	4

5. Detailed Syllabus

M. Sc. II (Sem- III) Physical Chemistry

PCH 301: Advanced Quantum Chemistry

Unit I: Basic Quantum Chemistry

Introduction. Exact solution of Schrödinger wave equation for rigid rotator, linear harmonic oscillator and hydrogen and hydrogen like atoms. Atomic orbitals, radial and angular shapes of atomic orbitals, ground and excited state energies, ionization potentials for hydrogen like systems. Transition dipole moment integral and selection rules for rotational, vibrational and electronic transitions.

Unit II: Ab initio methods

Self-consistent field (SCF) theory, Hartree-Fock (HF) method, quantum particles and their spins, properties of slater determinant, HF equations, restricted Hartree-Fock (RHF) and unrestricted Hartree-Fock (UHF) models, Fock matrix, HF calculations, Roothan-Hall equations, Koopman's theorem, Basis sets: Slater type orbitals (STO), Gaussian type orbitals (GTO), difference between STO and GTO, energy calculations using such orbitals for multielectron systems, classification

15 hrs.

of basis sets, minimal basis sets, energy calculations for H-atom using STO basis sets at different levels, double- and triple-zeta basis sets, valence-split basis sets, polarized basis sets, truncation and superposition errors, methods to overcome these errors. Correlation energy. Post Hartree-Fock methods: Configuration interactions, many body perturbation theory, Möller-Plesset perturbation, coupled cluster method. Introduction to various software packages for performing ab initio calculations.

Unit III: Density Functional Theory

15 hrs.

Basics of density functional theory (DFT): functionals, electron density and hole functions, fermi and coulomb holes, electron density as basic variable, Thomas-Fermi model, Slater's Approximation of Hartree-Fock Exchange, the Hohenberg-Kohn theorems, energy functionals, minimizing energy, orbitals and the non-interacting reference systems, the Kohn-Sham equations, computing the total energy, Exchange Correlation energy functional, Solving the Kohn-Sham equations: basis sets, Pseudopotentials, Plane waves, the self-consistent cycle, Density Functional Perturbation theory: basic formalism, first order energy derivative and atomic forces, second order.

Unit IV: Semiempirical Methods

Introduction, need of semi-empirical methods, zero differential overlap (ZDO) approximation. Variation principle, Secular determinant and secular equations. Hamiltonian in semi-empirical methods, Hückel molecular orbital theory – Assumptions of HMO theory, π -electron approximation, Hückel rule and aromaticity, HMO calculations for organic molecules, free valence index and prediction of chemical reactivity, use of molecular symmetry for simplification of HMO calculations. Neglect of differential overlap (NDO) method, complete neglect of differential overlap (CNDO), intermediate neglect of differential overlap (INDO), modified intermediate neglect of differential overlap (MINDO), neglect of differential overlap (MINDO). AM1, PM3, PM5, PM6 etc. methods, comparisons in various above-mentioned methods, limitations of semi-empirical methods. Introduction to various software packages for performing semi-empirical calculations.

Reference Books:

- 1. A. K. Chandra, Introductory Quantum Chemistry, 4th Edition, Tata McGraw-Hill, New Delhi, 1994.
- 2. D. A. McQuarrie, Quantum Chemistry, Viva Books, New Delhi, 2003.

- P. Atkins and R. Friedman, Molecular Quantum Mechanics, 4th Edition, Oxford University Press, New York, 2005.
- Leach, A.R. Molecular Modelling. Principles and Applications, 2nd Edition, Prentice-Hall, Harlow, England, 2001.
- K.I. Ramachandran, G. Deepa and K. Nimboori, Computational Chemistry and Molecular Modelling: Principles and Applications, Springer-Verlag, Berlin, Germany, 2008.
- 6. Becker, O.; MacKerell, A.D.; Roux, B.; Watanabe, M. eds. Computational Biochemistry and Biophysics, Marcel Dekker, New York, 2001.
- F. Jensen, Introduction to Computational Chemistry, 2nd Edition, John Wiley & Sons Ltd, West Sussex, England, 2007.
- D.B. Cook, Handbook of Computational Chemistry, Oxford University Press, New York, 1998.
- Fabio Finocchi, Density Functional Theory for Beginners: Basic Principles and Practical Approaches, 2011
- Wolfram Koch, Max C. Holthausen, A Chemist's Guide to Density Functional Theory, 2nd Edition, Wiley-VCH Verlag GmbH, Weinheim (Germany), 2001.
- 11. C. Fiolhais F. Nogueira M. Marques (Eds.), A Primer in Density Functional Theory, Springer-Verlag, Berlin, 2003.
- 12. P. Geerlings, F. De Proft, and W. Langenaeker, Conceptual Density Functional Theory, *Chem. Rev.* 2003, *103*, 1793-1873.

Course Outcomes (COs):

On completing the module students will be able to:

CO1: Learn concepts of atomic orbitals and their shapes, spectroscopic selection rules, ionization potentials, etc.

CO2: Learn advanced quantum methods such HF-SCF theory and post-HF methods and learners will be able to do accurate electronic energy and molecular structure calculations

CO3: Knowledge of the course will be used to do computer simulations to calculate molecular properties, NMR shift, IR and Raman spectra etc. for small to medium sized molecules or molecular assemblies.

CO4: Will familiarize in understanding and choosing the appropriate basis sets for electronic structure calculations with appropriate corrections through use of electron correlation methods CO5: Students will learn most advanced method of quantum mechanics i.e Density Function Theory for electron structure calculations

CO6: Learners will be capable of calculate the transition states, potential energy surfaces and reactions paths for chemical reactions using DFT method

CO7: Students can predict all the properties of materials at molecular level even for nanostructures, drugs, solids oxides, composites, solid electrolytes, electrode materials used in batteries and other electronic devices, etc.

CO8: For larger molecules like macrocycles, polymers, peptides etc., learners will be capable of replace or modify computationally demanding two-electron integrals through use semiempirical methods and parameterization tools used in these methods.

CO9: Knowledge of this course will make learners a potential candidate to work independently in any R&D laboratory or research laboratory or academic institutes of international repute.

PCH 302: Electrochemistry

UNIT–I: Equilibrium Properties of Electrolytes

Introduction, Debye – Huckel Theory of inter-ionic attraction, Ionic atmosphere, Time of relaxation, Relaxation and Electrophoretic effects, Debye – Huckel Onsagar equation, Validity of Debye – Huckel equation, factors influencing the degree of dissociation, , Debye – Falkenhagen effect, Wein effect, Debye Huckel limiting law equation, Qualitative and quantitative test of Debye Huckel limiting equation, Debye-Huckel Bronsted equations, Ionic mobility, Determination of dissociation constant by emf method, Experimental determination of ionic mobility, osmotic coefficient, Bjerrum theory, association constant, Numerical problems.

UNIT- II: Ion-solvent Interactions

Structure of water, hydration, heats of hydration of electrolytes, individual ions and their comparison, calculation of heats of hydration (Born, Van Arkel & de Boer, Bernal-Fowler methods), entropy of hydration and hydration numbers. Ion transport in solutions, diffusion, chemical potential and work of transport, Ficks laws, expressions for flux and diffusion coefficient. Ionic liquids: Introduction, difference between electrolytes and ionic liquids, diffusion in fused salts, viscosity and diffusion coefficient in molten salts.

UNIT-III: Electrode reactions

Electrified interface, electron transfer under interfacial electric field, symmetry factor, electrode at equilibrium, exchange current density, over potential, Butler-Volmer equation, high field and low field approximations, Tafel equations, Multistep electrode reactions; Marcus microscopic

15 hrs.

15 hrs.

model of electron transfer. Electrode kinetics of semiconductor/ solution interface; n and p type semiconductor, current-potential relation of n and p type semiconductors Electrocatalysis: Influence of various parameters on water splitting, HER and OER and Application of cyclic voltammetry for characterization of various electrochemical processes, Electrochemical instrumentations. Bioelectrochemistry: Nerve impulses, Membrane potentials, Nernst-Planck equation, Hodgkin-Huxley equations, electrochemical impedance spectroscopy.

UNIT-IV: Fuel cell and Corrosion

15 hrs.

Fuel cell: Significance of fuel cells, Hydrogen – oxygen fuel cells, hydrocarbon - air fuel cell, alkaline fuel cells, Phosphoric acid fuel cell (PAFC), Proton exchange membrane fuel cells (PEMFC), Solid oxide fuel cells, Molten Carbonate Fuel Cell (MCFC), Alkaline Fuel cell (AFC), Solid Polymer Fuel Cell (SPFC) and applications. Corrosion: Introduction, Comparison between dry and wet corrosion, Factors affecting corrosion: Nature of the metal, Nature of the corroding environment, Types of corrosion, Prevention of corrosion: Material selection & Design, protective coatings, corrosion inhibitors.

Reference Books:

1. An Introduction to Electrochemistry by Samuel Glasstone, East west press riveted limited (2005).

2. Callister's Material Science and Engineering adapted by R. Balasubramaniam, Wiley India(p) Ltd.

3. Electrolytic Solutions, by R. A. Robinson and R. H. Strokes

4. Physical Chemistry by P. W. Atkins. ELBS.

5. Electrochemical Methods: Fundamentals and Applications, Bard, A. J. Faulkner, L. R., 2nd Ed., John Wiley & Sons: New York, (2002).

6. Electrochemical Science and Technology: Fundamentals and Applications, Oldham, K. B.,

Myland, J. C. and Bond, A. M. John Wiley & Sons, Ltd. (2012).

7. Modern Electrochemistry 2A: Fundamentals of Electronics, 2nd Ed., Springer

(2001).Bockris, J. O' M., Reddy, A. K. N. & Gamboa-Aldeco, M. E.

8 Electrochemistry, Brett, C. M. A. & Brett, A. M. O., Oxford University Press (1993).

9. Principles of Electrochemistry, John Wiley & Sons: NY (1993).

10. Fundamentals of electrochemistry, Bagotsky, V.S., 2nd Ed. Wiley – Interscience, (2006)

Hamann, Carl H., Hamneff, Andrew & Vielstich, Wolf., Electrochemistry, 2nd Ed.(2007) 47.

Fuel Cell Systems Explained Second Edition by James Larminie Andrew Dicks, John Wiley
& Sons Ltd, The Atrium, Southern Gate, Chichester, West Sussex PO19 8SQ, England.

Course Outcomes (COs):

Upon course completion the student is able to:

CO1: Learning the Debye-Huckel theory and it apply for electrolytic solutions. Students will able to learn experimental determination of ionic mobility, osmotic coefficient by using Debye-Huckel theory.

CO2: Students will learn how to calculate hydration number and heat of hydration by using Born, Van Arkel & de Boer and Bernal-Fowler methods. Learning the different properties of the Ionic liquids and flux and diffusion coefficient.

CO3: Learning the different electrode reactions, exchange current density, over potential, Butler-Volmer equation, high field and low field approximations. Students will able to learn electrode kinetics of semiconductor/ solution interface.

CO4: Students will able to learn the significance of fuel cells and different types of electrochemical cells and their applications. They learn the types of the corrosion and their applications in various industries.

PCH 303: Molecular Structure-I

UNIT- I: Symmetry properties of molecules and group theory 15 hrs.

Symmetry elements, symmetry operations and point groups, properties of group, symmetry operations as a group, multiplication table. Classes of symmetry operations, basis, representative and matrix representations of operations. Reducible and irreducible representations, orthogonality theorem. Properties of irreducible representations. Constructions of character table for point groups. Explanations for the complete character table for a point group. Representations of vibrational modes in nonlinear molecules. Infrared and Raman activities of normal modes of vibrations.

UNIT– II: Introduction of spectroscopy and Rotational Spectra 15 hrs.

Characterization of electromagnetic radiation. The qualification of energy. Regions of Spectrum, transition probability, the width and intensity of spectral transitions. Classification of molecules according to their moment of inertia. Rotational spectra of rigid and non rigid diatomic molecules.

The intensities of spectral lines. The effect of isotopic substitution. Polyatomic and symmetric top molecules. The stark effect.

UNIT- III: Infrared spectroscopy and Raman Spectroscopy

15 hrs.

15 hrs.

Diatomic molecules: 1) Molecules as harmonic oscillator, Morse potential energy function, vibrational spectrum, fundamental vibrational frequencies. Force constant, zero point energy, isotope effect. The anharmonic oscillator, the diatomic vibrating rotator, the interactions of rotations and vibrations. Polyatomic molecules: Fundamental vibrations and their symmetry, overtone and combination frequencies. The influence of rotations and molecular spin on the spectra of polyatomic molecules. Analysis by Infrared techniques. Raman Spectroscopy: Rayleigh scattering. Raman Scattering, classical and quantum theories of Raman effect. Rotational Raman Spectra for linear and symmetric top molecules. Vibrational Raman Spectra, rotational fine structure. Polarization of light and the Raman effect. Structure determination from Raman and Infra-red spectroscopy.

UNIT – IV: Electronic Spectroscopy

General nature of band spectra. Beer- Lambert Law integrated absorption coefficient and oscillator strength. Term symbols for atoms and molecules. The hydrogen atom and hydrogen like species spectrum. Sequences and progressions, the vibrational course structure and rotational fine structure of electronic band. The Franck-Condon principle, dissociation energy and dissociation products. Birje-Sponer extrapolation. The fortrat diagram. Predissociation, classification of electronic states. The spectrum of molecular hydrogen. Electronic spectra of polyatomic molecules. Chemical analysis by electronic spectroscopy. (d-d) and (-n*) transitions. Photochemical mechanism of vision.

Reference Books:

1. Fundamental of molecular spectroscopy by C. N. Banwell, E. M. McCash, Vth Edn.,

Tata McGrew Hill(2013).

- 2. Physical Chemistry by P. W. Atkins, J. D. Paula, IXth Edn., Oxford University Press (2010).
- 3. Chemical Applications of Group Theory, F. A. Cotton, 3rd Edn., Wiley-India(2009).
- 4. Molecular Symmetry and Group Theory by R. L. Carter, John-Wiley & Sons Inc.(1998)
- 5. A Text Book of Physical Chemistry by K. L. Kapoor, IVth Edn., Macmillan (2011).
- 6. Symmetry & spectroscopy of molecules by K. Veera Reddy, IInd revised Edn., New Age International Publishers (2009)

7. Intruduction to spectroscopy by D. L. Pavia, G. M. Lapmann, G. S. Kriz, IIIrd Edn., Thomson(2006).

8. Molecular Structure and Spectroscopy by G. L. Aruldhas, Prentice-Hall of India Pvt. Ltd. (2006).

Course Outcomes (COs):

On completing the module students will be able to:

CO1: The student will be able to represent the properties of a molecule in a mathematical form.

CO2: The unit deals with determination of molecular parameters like bond length spectroscopically.

CO3: the student will be capable of predicting the basic structure of a compound.

CO4: the student will be able to understand the electronic structure stabilizing the given molecule.

PR-PCH305: Physical Chemistry Practicals (2 Cr) 60 hrs.

- 1. Determination of stability constant of ferric thiocyanate complex.
- 2. To determine stoichiometry and stability constant of ferric-salicylate complex by Job's Method and mole ratio method spectrophotometrically.
- 3. Determination of stoichiometry and instability constant silver ammonia complex.
- 4. Determination of transport number of H⁺, Na⁺, K⁺ etc. ions using moving boundary method.
- 5. Determination of the critical micelle concentration of a given surfactant in aqueous and aqueous salt solutions.
- 6. Determination of equivalent conductance at infinite dilution and dissociation constant for weak acid using Kohlrausch Law of independent ionic mobility.
- 7. pH-metric determination of dissociation constant of carbonic acid.
- 8. Cryoscopic determination of molecular weight and state of organic acids in nonaqueous volatile solvents.
- 9. Determination of order of reaction for iodination of acetone catalyzed by acid with reference to acetone, iodine and acid catalyst.
- 10. Determination of apparent and partial molar volumes of 1:1 electrolyte in aqueous solutions using pyknometric method of density measurements.
- 11. Structure drawing, Geometry optimization and Single-point energy calculations for small molecules using minimal basis sets.

- 12. Structure drawing, Geometry optimization and Single-point energy calculations for small molecules using correlation consistent basis sets.
- 13. Semi-empirical and quantum mechanical determination of thermochemical properties of small molecules.
- 14. Statistical representation of given experimental data: Estimation of errors in measured and derived properties, reporting data with appropriate significant figures, graphical representation of data with x- and y-error bars.
- 15. Determination of molecular properties of small gaseous molecules from rovibrational spectra.
- 16. Determination of indicator constant and isosbestic point of an indicator.
- 17. Determination of Thermodynamic Parameters for electrochemical reactions: To determine ΔG^0 , ΔH^0 and ΔS^0 for the formation of 1 mole of cadmium in 1 wt. % amalgam at 25 °C.
- 18. Determination of isoeletric points and dissociation constants for neutral, acidic and basic amino acids using pH-metric technique.
- 19. Cryoscopic determination of mean activity coefficient of 1:1 electrolytes in aqueous solutions.
- 20. Study of the effect of ionic strength on the reaction between persulphate and iodide by visual method.
- 21. Determination of molar enthalpy of solution, molar enthalpy of dilution and partial molar heat content of components in aqueous solutions.
- 22. Structure drawing, Geometry optimization and Single-point energy calculations for small molecules using minimal basis sets.
- 23. Structure drawing, Geometry optimization and Single-point energy calculations for small molecules using correlation consistent basis sets.
- 24. Electronic structure calculations for small molecules and their aggregates.
- 25. Calculation of vibration spectra using abinitio techniques.
- 26. Structure and properties of transition states from DFT calculation.
- 27. Determination of thermodynamic properties from Molecular dynamic simulations of some simple systems.

Along-with above experimental and computational lab work, additional new experiments from computational chemistry as well as from experimental techniques will be given whenever required and found necessary for enhancing the knowledge and skill of the students.

NOTE: Student should perform their practical work in the laboratory minimum 15 days in one semester for 2 credits.

Course Outcomes (COs):

- CO1: The students will acquire hands on training for conducting the representative experiments for the analysis of wide variety of samples of inorganic, organic and physical approaches by qualitative and quantitative analysis
- CO2: Student would learn the sample preparation and characterization for purity and qualitative and quantitative analysis of samples.
- CO3: Students will have good experimental skills for separation and estimation of amount of metal, metal ions in given samples.
- CO4: Students will be acquainted with the separation and estimation of organic compounds in given samples.

RP-PCH306: Research Project (4 Cr)

See Annexture-I for details.

M. Sc. II (Sem - IV) Physical Chemistry

PCH 401: Thermodynamics and Molecular Modelling

Unit I: Modern Theoretical Principles

Exact and inexact differential expressions in two variables. Total differentials. Techniques of partial differentiations. Transformation of variables. Maxima and minima. Integrating factors, Paff differential equations, Caratheodary's theorem. Legendre transformations. Derivation of thermodynamic identities. The second law of thermodynamics, classical formulations, mathematical consequences of second law. Entropy changes, Clausius inequality. Free energy concept. General condition of equilibrium. Thermodynamic potentials.

Unit II: Statistical Thermodynamics

15 hrs.

Ensembles, ensemble average and time average of the property, ergodic hypothesis, partition functions and thermodynamic properties, classical and quantum statistics, properties of photon gas, thermodynamic properties bosons, use of quantum statistics for evaluation of absolute entropies, condensation of helium, Fermi energy, electron gas in metals. Heat capacity of solids, Einstein and Debye specific heat equations. Characteristic temperatures. Debye T^3 law.

Unit III: Molecular Mechanics and Molecular Dynamic Simulation Methods 15 hrs.

Introduction, microscopic and macroscopic properties, time scale of chemical/biological process, the Morse potential model, harmonic oscillator model, force fields development, various energy terms and non-covalent interactions included in force fields, Lennard-Jones type and truncated Lennard-Jones potentials, commonly used force fields, parameterization, advantages and limitations of Force Field Methods, molecular dynamics methods, neighbor searching, Trotter decomposition, cut-offs, temperature and pressure coupling methods, integration algorithms: Verlet algorithm, Leap-frog algorithm, Velocity Varlet, Beeman's algorithm, Constraint algorithms: shake, Lincs, etc., topology files, energy minimization: steepest descent method, conjugate gradient method, L-BFGS. Solvent models, Solvation, implicit and explicit solvation, heating, equilibration and production dynamics, trajectory analysis, particle mesh Edward dynamics, boundary conditions, Exclusions and 1-4 interactions, replica exchange method, conformational analysis, normal mode analysis, free energy calculation: free energy perturbation method, thermodynamic integration method, thermodynamic cycles for free energy calculations, determination of hydration/solvation free energy, protein folding free energy, protein-ligand binding free energy etc. Software packages for performing Molecular dynamic simulation as well as for visualization and analysis trajectories.

Unit IV: Non-equilibrium thermodynamics

15 hrs.

Conservation of mass in closed and open systems, conservation of energy in closed and open systems. Law of increasing entropy. Non-adiabatic processes and Clausius inequality, steady state. Thermodynamic equations of motions. Chemical and electrochemical affinities. Coupling reactions. Rates and affinities. Generalized fluxes, forces and their transformation. Phenomenological equations and coefficients. Concepts of reciprocity relations and Onsager theorem of microscopic reversibility. Entropy production in closed and open systems. Entropy production due to heat flow. Chemical potentials. Diffusion, electromotive force, electro-osmosis, thermoelectric effect and other reactions involving cross relations. Saxen's relations.

Reference Books:

- 1. S. N. Blinder, Advanced physical Chemistry, The Macmillan Company, 1967.
- 2. L. K. Nash, Elements of statistical thermodynamics, 2nd Edition, Addison Wesley, 1974.
- 3. T.L. Hill, An Introduction to Statistical Thermodynamics, Addison-Wesley, 1960.
- 4. S. Glasstone, Theoretical Chemistry: An introduction to quantum mechanics, statistical mechanics, and molecular spectra for chemists, D. Van Nostrand Company, Inc., 1944.
- 5. D. A. McQuarrie and J. D. Simon, Physical Chemistry: A molecular Approach, Viva Books, New Delhi, 1998.
- Allen, M. P., Tildesley, D. J. Computer Simulations of Liquids, Oxford: Oxford Science Publications. 1987.
- 7. Frenkel, D.; Smit, B. Understanding Molecular Simulation: From Algorithms to Applications, 2nd Edition, Academic Press, San Diego, 2002.
- 8. K.I. Ramachandran, G. Deepa and K. Nimboori, Computational Chemistry and Molecular Modelling: Principles and Applications, Springer-Verlag, Berlin, Germany, 2008.
- F. Jensen, Introduction to Computational Chemistry, 2nd Edition, John Wiley & Sons Ltd, West Sussex, England, 2007.
- 10. Schlick, T. Molecular modelling and simulation: an interdisciplinary guide, Springer-Verlag New York, Inc., Secaucus, NJ, USA, 2002.
- D.B. Cook, Handbook of Computational Chemistry, Oxford University Press, New York, 1998.
- 12. Online Manuals for simulation and visualization packages such as GROMACS, VMD, NAMD, AMBER, TINKER, etc.
- I. Prigogine, Introduction to Thermodynamics of Irreversible Processes, Wiley, New York, 1968.
- 14. R.P. Rastogi, Introduction to Non-equilibrium Physical Chemistry: Towards Complexity and Non-linear Science, Elsevier, Oxford, 2008.

Course Outcomes (COs):

After completion of course student will able to learn

CO1: Students with weaker background in mathematical principles will learn how to explore the scientific findings with mathematical models and advance it further.

CO2: Learn principles of statistics to understand and estimate bulk thermodynamic properties of materials.

CO3: Understand how microscopic properties where quantum effects are predominant can be correlated to macroscopic properties where classical thermodynamics is important through ensemble theories and statistical distribution laws.

CO4: Through these studies, students will be able to evaluate the thermodynamic properties of systems of quantum particles such as bosons and fermions.

CO5: Knowledge can be used to utilize the classical and statistical thermodynamic principles for computer simulation of real-life processes through molecular dynamic simulations.

CO6: Learn techniques of MD simulations to evaluate the molecular properties and structural features for understanding the functions of biopolymers and its applications in drug design, material design, protein chemistry, polymer industry, etc.

CO7: Students will learn applicability of principles of thermodynamics where irreversible effects or near equilibrium phenomena exist.

CO8: Students will gain knowledge about science behind the industrially important phenomena like production of electricity from thermal sources, Peltier effects, electrophoresis, osmosis, thermos-diffusion, thermos-conductivity etc.

PCH 402: Chemical Kinetics

UNIT-I: Collision Theory

Collision Theory: Definition, Formulation of the total collision rate, p factor, Reactive collisions, Contour diagrams for scattering of products of a reaction, Forward scattering: the stripping or grazing mechanism, Backward scattering: the rebound mechanism, Scattering diagrams for longlived complexes, Steady State Approximation Collision theory of gas reaction, collision frequency. The rate constant, molecular diameters, collision theory vs. experiment.

UNIT – II: Transition State Theory

Transition State Theory: Transition state theory, configuration and potential energy, Properties of the potential energy surface relevant to transition state theory, An outline of arguments involved in the derivation of the rate equation, Use of the statistical mechanical form of transition state theory, Comparisons with collision theory and experimental data. Thermodynamic Formulations of Transition State Theory: Determination of thermodynamic functions for activation, the partition function form and the Thermodynamic form of transition state theory, Typical approximate values of contributions entering the sign and magnitude of $\Delta S^{\#}$, Unimolecular Theory: Manipulation of experimental results, Physical significance of the constancy or otherwise

15 hrs.

of k1, k-1 and k2, Physical significance of the critical energy in unimolecular reactions, Physical significance of the rate constants k1, k-1 and k2. Lindemann, Hinshelwood, theory, Kassel and Slater Theory.

UNIT-III: Kinetics of Surface Reactions

Review of adsorption isotherms, Thermodynamics and statistical mechanics of adsorption, Structure of solid surfaces and adsorbed layers: Detailed structural studies, Induced Heterogeneity, Mechanism of surface reactions: Kinetic effects of surface heterogeneity, Kinetic effects of interaction Unimolecular surface reactions: Inhibition, Activation Energies, Bimolecular surface reactions: Reaction between two adsorbed molecules reaction between a gas molecule and an adsorbed molecule, Adsorption of two gases without mutual displacement, Inhibition, Activation energies, Parahydrogen conversion, Combination and formation of atoms at surfaces, Exchange reactions, Addition of hydrogen to ethylene, Transition state theory of surface reactions: rates of chemisorption, rates of desorption, Unimolecular surface reactions, bimolecular surface reactions, comparison of homogeneous and heterogeneous reaction rates, Problems.

UNIT- IV: Fast Reactions and Organic Reaction Mechanisms 15 hrs.

Linear free energy relationships: Hammett plots Hammett equation, substituent and reaction constants and their physical significance, calculation of k and K values, Yukawa-Tsuno equation. Taft equation, steric parameters Solvent effects, Grunwald-Winstein equation. Kinetics of Fast reactions: Relaxation techniques, pressure jump and temperature jump methods, NMR relaxation, flash photolysis and molecular beam methods.

Reference Books:

- 1. Chemical Kinetics by K. J. Laidler, Third Edition, Pearson.
- 2. Kinetics and Mechanism by A. A. Frost and R. G. Pearson.
- 3. Fast Reactions by Haque.
- 4. Theory of chemical reaction rates by K. J. Laidler, McGrew Hill, New York, 1969.
- 5. Physical Chemistry by P.W. Atkins
- 6. Mechanism of Inorganic Reactions by F. Basolo John Wiley & Sons 1967.
- 7. A Guidebook to Mechanism in Organic Chemistry, Peter Sykes, Orient Longmann, 2003.

Course Outcomes (COs):

After completion of course student will able to learn

CO1: Students can understand the basic principles of Kinetics

CO2: Students can learn different theories of rates of reaction

CO3: Learn from fundamental to advanced theories and applications of chemical kinetics

CO4: Different methods of study of dynamics of fast reaction mechanism

CO5: Different mechanistic aspects of surface reaction and industrial applications

CO6: Reaction mechanism and photocatalytic applications of materials

CO7: Linear free energy equation and substitutions on aromatic group

CO8: Students learn effect different equations expressions expressing reaction constant and substitution constant.

PCH 403: Molecular Structure-II

UNIT – I: The Electrical and Magnetic Properties of Molecules 15 hrs.

Electric dipole moment of molecule, polarization of a dielectric, polarizability of molecules, Clausius-Mossotti equation. Debye equation. limitation of the Debye theory, determination of dipole moment from dielectric measurements in pure liquids and in solutions.

Diamagnetism and paramagnetism. Volume and mass susceptibilities. Lengevins classical theory of diamagnetism and paramangnetism Atomic and ionic susceptibility. Pascal constants, Curie - Weiss law. Van Vleck general equation of magnetic susceptibility. Determination of magnetic susceptibility.

15 hrs.

UNIT – II: Nuclear Magnetic Resonance Spectroscopy

The nature of spinning particles, interaction between spin and a magnetic field. Population of energy levels, The Larmor precession. relaxation times. the meaning of resonance and the resonance condition. NMR experiment, significance of shielding constants and chemical shift. The origin and effect spin - spin coupling, factors affecting chemical shift, chemical analysis by NMR. Exchange phenomena, 13C NMR spectroscopy, double resonance and nuclear-Overhauser effect.

UNIT – III: Electron Spin Resonance Spectroscopy and Mossbauer Spectroscopy 15 hrs.

Electron spin and Magnetic moment, Resonance condition in ESR and significance of 'g' value. ESR spectra of organic free radicals, McConnel relation, Electron Exchange reactions, applications of ESR, B) Mossbauer Spectroscopy (7) Basic principle of Mossbauer spectroscopy, hyperfine structure, quadrupole splitting, instrumentation and applications of Mossbauer spectroscopy, Problems related to Mossbauer spectra.

UNIT – IV: Mass Spectroscopy

Introduction, basic theory, instrumentation-single focusing, double focusing, quadrupole mass filter, TOF instruments. Methods pf generation of positively charged ions-electron impact ionization, chemical ionization, fast atom bombardment (FAB), matrix assisted laser desorption ionization (MALDI).

Resolving power, base peak, molecular ion peak, meta stable peak, isotopic peaks, calculations of percentage intensity of (m+1) and (m+2) peaks. Exact molecular mass, molecular formula, hydrogen deficiency index, preliminary analysis of structure. Modes of fragmentation-fragmentation rules.

Reference Books:

1. Fundamental of molecular spectroscopy by C. N. Banwell, E. M. McCash, Vth Edn.,

- Tata McGrew Hill (2013).
- 2. Physical Chemistry by P. W. Atkins, J. D. Paula, IXth Edn., Oxford University Press (2010).
- 3. Introduction to molecular spectroscopy by G. M. Barrow.
- 6. Introduction to Magnetic resonance by A. Carrrington and A. D. McLachlan. Harper and Row.
- 8. Introduction to Magnetochemistry by Earnst Shaw. Academic Press
- 9. Electrical and optical properties of molecular behavior by M. Davies, Pergmon press.
- 10. Polar molecules by P. Debye, Dover publications.
- 11. A Text Book of Physical Chemistry by K. L. Kapoor, IVth Edn., Macmillan (2011).

Course Outcomes (COs):

After completion of course student will able to learn

CO1: the unit deals with the understanding of behaviour of various materials in presence of applied electrical and magnetic fields.

CO2: the student will be able to predict structure of the given compound.

CO3: the student will be able to understand behaviour of electrons and nucleus of a given molecule in presence of an external force like magnetic field and iinstrumentation and applications of the Mossbauer spectroscopy.

CO4: Students will learn Instrumentation and applications of the Mass spectroscopy.

RP-PCH405 Research Project (6 Cr, 180 Hrs) 150 Marks

See Annexture-I for details.

NOTE: Study tour is part of your syllabus for M.Sc. Part- II. Students shall visit Chemical Industries in India.

Name of Program: M. Sc. Analytical Chemistry

Analytical Chemistry is a pervasive and a key subject not only for Chemistry, but all the branches of Science, Engineering and Technology which involves Chemistry. It is an experimental science and students need to be trained in theory and practical dealing with fundamental and advanced analytical skills of conventional analysis and instrumental analysis so as to get expertise in doing fine experiments and handle sophisticated instruments.

The M.Sc. Analytical Chemistry program offered by Shivaji University is a **Two Years** full time program. The first and second semester gives general background of analytical chemistry and its importance to all the branches of Chemistry to make a good theoretical background of students. The semester third and fourth is totally assigned to analytical chemistry and it covers most of the fundamental and advance aspects of modern analytical chemistry. In order to make students more careers oriented and nurturing their scientific temperaments, students will get exposure to the depth of core understanding of various dimensions of analytical chemistry during these two years the study.

1. Program Outcomes (POs):

- PO1. The M.Sc. analytical chemistry program at Shivaji University, Kolhapur provides the key knowledge base and laboratory resources to prepare students for careers as professionals in the field of chemistry and particularly in analytical chemistry enabling them to interface not only with various branches of chemistry (organic, inorganic, physical, biological, industrial, environmental, pharmaceuticals etc) but also with the related fields, and for professional courses and areas of research including medical, forensic, food, agriculture, dental, law, intellectual property, business programs etc.
- PO2. Students will be able to solve various problems by identifying the essential parts of a problem, formulate strategy for solving the problem, applying appropriate techniques to arrive at a solution, test the precision and accuracy of the solution and interpret the results.
- PO3. Students will be able to acquire domain specific knowledge and technical skills needed for employment in industries, teaching fields and pursue research. Students will be skilled in problem solving, critical thinking and analytical reasoning.
- PO4. Students will be able to apply the fundamental knowledge to address the cross-cutting issues such as sustainable development.

- PO5. Students will get perfect insight into qualitative and quantitative analytical chemistry and research ethics for production of quality research.
- PO6. Students will be able to communicate effectively i.e. being able to articulate, comprehend and write effective reports, make effective presentations and documentation and capable of expressing the subject through technical writing as well as through oral presentation.

2. **Program Specific Outcomes (PSOs):**

- PSO 1. Students will be able to prepare and qualify subject specific competitive exams like NET, SET and GATE and also other general public administration exams like M.P.S.C. and U.P.S.C. etc. exams.
- PSO 2. Student will be able to utilize the knowledge and analytical skills in QA-QC and R&D departments in almost all the industries enabling them to secure jobs where analytical chemistry is the core requirement to ensure and ascertain the quality of the product.
- PSO 3. Students will have opportunity for higher education leading to Ph.D. program.
- PSO 4. Students will be able to explore contemporary research in chemistry and allied fields of science and technology, collaborate in team projects, and communicate the results of scientific work in oral, written and electronic formats to both scientists and the public at large.
- PSO 5. Students can start their own laboratories/startups/ chemical industry/ business (entrepreneurship).
- PSO 6. Students will be able to interprete data from the state of art Analytical instruments for ascertaining the product/material.

3. Framework of NEP 2.0 as per NEP-2020 for M. Sc. Degree in Analytical Chemistry

Class	SEM	Level	Mandatory Subject	Elective Choose any One	RM (4 Cr)	OJT/FP (4 Cr)	RP	Cumm. Cr	Degree
M.Sc. II	Ш	6.5	ACH.301 (4Cr)	E-ICH.304 (4Cr) OR			RP-ACH.	22	M.Sc. Degree
			ACH.302 (4Cr)	E-OCH.304 (4Cr) OR			306 (4 Cr)		in Analytical
			ACH.303 (4Cr)	E-PCH.304 (4Cr) OR E-ACH.304 (4Cr) OR					after 3/4 yr.
			PR-ACH305 (2 Cr)						UG
	IV	6.5	ACH.401 (4Cr)	E-ICH.404 (4Cr) OR			RP-ACH	22	
			ACH.402 (4Cr)	E-OCH.404 (4Cr) OR E-PCH 404 (4Cr) OR			405 (6 Cr)		
			ACH.403 (4Cr)	E-ACH.404 (4Cr) OR					
Cum. Cr. I	For 1 Y Degree	ear PG	26 Cr	8 Cr			10	44	

3. Course Structure: M.Sc. Part-II, Analytical Chemistry

Semester III

Major Mandatory

Course Code	Course Title	Credits
ACH301	Advanced Analytical Techniques	4
ACH302	Organo Analytical Chemistry	4
ACH303	Electroanalytical Techniques in	4
	Chemical Analysis	
PR-ACH305	Analytical Chemistry Practicals- V	2
RP-ACH306	Research Project	4

Major Elective (Choose any one)

Course Code	Course Title	Credits
E-ICH304	Organometallic and Bioinorganic Chemistry	4
E-OCH304	Drug and Heterocycles	4
E-PCH304	Solid State Chemistry	4
E-ACH304	Environmental Chemical Analysis and Control	4

Semester IV

Major Mandatory

Course Code	Course Title	Credits
	Madam Sananatian Mathad in Analysis	4
ACH401	Modern Separation Method in Analysis	4
ACH402	Organic Industrial Analysis	4
ACH403	Advanced Methods in Chemical Analysis	4
RP-ACH405	Research Project	6

Major Elective (Choose any one)

Course Code	Course Title	Credits
E-ICH404	Energy and Environmental Chemistry	4
E-OCH404	Applied Organic Chemistry	4
E-PCH404	Surface Chemistry	4
E-ACH404	Applied Analytical Chemistry	4

5. Detailed Syllabus

M.Sc. Part-II (Sem-III) Analytical Chemistry

ACH301: ADVANCED ANALYTICAL TECHNIQUES

Unit-I: Advances in Mass Spectrometry-A

15 hrs.

Introduction to Mass spectrometry, diagram of a mass spectrometer and Instrumentation, principles, history, concept of ion free path, classification of mass spectrometry based on nature of compound to be analyzed and the ion sources viz. Electron impact (EI), chemical ionization (CI), Fast ion or atom bombardment ionization (FID/FAB), field desorption (FD), laser desorption ionization (LDI), plasma desorption ionization (PDI), thermospray ionization (TSI), electrospray (ESI), atmospheric pressure ionization, Inductively couple plasma (ICP) etc. Mass Analyzers, Quadrupolar Analyzers, Quadrupole ion trap or Quistor, Ion trap detector, development of high –Mass, High-resolution ion trap, tandem mass spectrometry in the ion trap, time of flight analyzer, magnetic and electromagnetic analyzer, ion cyclotron resonance and FT-MS, and detectors

Unit-II: Introduction to Nanotechnology and Nano Chemistry

Definition of nanomaterials and nanotechnology, significance of nanotechnology, size and properties, types of nanomaterials like 0D (quantum dots), 1D, 2D and 3D, introduction to physical, chemical and biological synthesis of nanomaterials with suitable examples, top down and bottom-up approach, chemical synthesis of nanomaterials-Different types and processes for synthesis of nanomaterials using wet chemical approaches. Fabricating nanomaterials with different morphology intended for specific applications. Applications of Nanotechnology.

Unit-III: Advanced Instrumentation Techniques-A

Scanning Electron Microscope (SEM) - Introduction, principle, instrumentation, applications Transmission Electron Microscope (TEM) - Introduction, principle, instrumentation, applications Electron Dispersion Spectroscopy (EDS) - Introduction, principle, instrumentation, applications Energy Dispersive X-ray Analysis (EDAX) - Introduction, principle, instrumentation, applications, applications.

Scanning Tunneling Microscopy (STM) - Introduction, principle, instrumentation, applications Atomic Force Microscopy (AFM) - Introduction, principle, instrumentation, applications Practical applications and examples in analytical chemistry and research.

Unit-IV: Advanced Instrumentation Techniques-B

Raman Spectroscopy- Introduction, principle, instrumentation, applications X-Ray Fluorescence Spectroscopy (XFS) - Introduction, principle, instrumentation, applications Electron Spin Resonance Spectroscopy (ESR)- Introduction, principle, instrumentation, applications. X-Ray Photoelectron Spectroscopy (XPS)- Introduction, principle, instrumentation, applications Auger Electron Spectroscopy - Introduction, principle, instrumentation, applications, Secondary Ion Mass Spectrometry (SIMS)- Introduction, principle, instrumentation, applications Practical applications and examples in analytical chemistry and research.

Reference Books:

- 1. E. De. Hoffmann, J. Charette, V. Stroobant, Mass Spectroscopy: Principles and Applications, John Wiley & Sons, Masson, Paris 1996.
- 2. J. H. Gross, Mass Spectroscopy: A Text book, Springer-Verlag Berlin 2004.
- 3. C. G. Herbert, R. A. W. Johnstone, Mass Spectrometry Basics, CRC Press, Boca Raton, Florida, 2002.
- 4. K. Benjamin: Mass Spectrometry
- 5. A. I. Vogel: A text book of Quantitative inorganic Analysis, Lonqmans.

15 hrs.

15 hrs.

- 6. G. H. Morrison and H, Freiser: Solvent Extraction in Analytical Chemistry (John Wiley New York, 1958)
- 7. Willard, Merrit and Settle: Instrumental Methods of analysis.
- 8. Principles of instrumental analysis- Holler, Skoog and Crouch
- 9. Instrumental methods of Chemical analysis-H. Kaur
- 10. Bhushan, Bharat 2004. Handbook of Nanotechnology. Springer.
- Niemeyer, C.M. & Mirkin, C.A. 2004. Nanobiotechnology- Concepts, Applications and Prespectives. Wiley-VCH Verlag.
- Zander, C., Enderlein, J. & Keller, R.A. 2002 Single Molecule Detection in Solution. Wiley- VCH Verlag.
- 13. Avouris, P, Klitzing, K. Von, Sakaki, H. & Wiesendanger, R. 2003 NanoScience and Technology
- 14. Series. Scanning Probe Microscopy- Analytical Methods (R. Wiesendanger eds), Springer.
- 15. Instrumental Analysis by Skoog
- Nanochemistry, a chemical approach to nanomaterials, G. A. Ozin, and A. C. Arsenault, RSC Publishing, Cambridge, 2005. ISBN 0-85404-664-X.

Course Outcomes (COs):

CO 1: Develop knowledge of fundamental, instrumentation and working of state of art instrumental analytical techniques, effective use and choice of technique, written and/or oral communication of the concepts of analytical chemistry which will be useful as analytical chemist and R&D.

CO 2: Acquire knowledge of mass spectrometry, type of MS, ionization types and specific practical applications of MS.

CO 3: Acquire knowledge of basics of nanochemistry, nanomaterials and nanotechnology and application orientated synthesis and characterization of nanomaterials.

CO 4: This course gives wide understanding about the instrumental analytical techniques (SEM, TEM, EDS, STM, AFM, Raman, XFS, ESR, XPS, AES, SIMS etc.)employed for qualitative and quantitative analysis for contemporary research.

ACH302: Organo Analytical Chemistry

UNIT–I: Hyphenated Techniques

Advanced techniques of analysis: UV-Visible, IR, 1H-NMR (Recapitulation), 13CNMR, Mass spectrometry (Basic fundamentals of mass spectrometry, ionization, advanced organic analysis examples); Problems related to structure determination and applications of spectroscopic techniques as analytical tools.

UNIT-II: A) Drug Analysis

Introduction to drugs, their classification, sources of impurities in pharmaceutical raw materials such as chemical, atmospheric and microbial contaminants etc. Limit tests: Limit test for impurities for Pb, As, Fe, Se, etc. Estimation of moisture (K-F method), halide (Schnoiger's oxygen flask method), sulfate, boron, etc. Analysis of commonly used drugs such as antihistamines, sulfa drugs, barbiturates, etc. using non-aqueous titrations, sodium nitrite titrations, differential UV methods, colorimetric and fluorimetric methods of analysis.

B) Analysis of vitamins

Analysis of vitamins (thiamine, ascorbic acid, Vit. A, Vit. B6, Vit. K) and hormones (progesterone, oxytocin, insulin) chemical, instrumental and biological assay, wherever applicable.

UNIT – III: A) Clinical Analysis

Biological significance, analysis of assay of enzymes (pepsin, monoamine, oxidase, tyrosinase), Composition and detection of abnormal level of certain constituents leading to diagnosis of diseases. Sample collection and preservation of physiological fluids, analytical methods to the constituents of physiological fluids (blood, urine and serum). Blood- Estimation of glucose, chlolesterol, urea, hemoglobin and bilirubin, Urine- urea, uric acid, creatinine, calcium, phosphate, sodium, potassium and chloride.

B) Body fluid analysis

Composition and detection of abnormal level of certain constituents leading to diagnosis of diseases. Sample collection and preservation of physiological fluids, analytical methods to the constituents of physiological fluids (blood, urine and serum) Blood-Estimation of glucose, chlolesterol, urea, hemoglobin and bilirubin Urine- urea, uric acid, creatinine, calcium, phosphate, sodium, potassium and chloride.

08 hrs.

05 hrs.

07 hrs.

15 hrs.

UNIT–IV: A) Pesticides Analysis

Introduction, classification of pesticides, sampling, sample pretreatment and processin g, analysis of DDT, gammexane, endosulphan, zinab, ziram, malathion, thiram, thiometon, simazine and chloridane. Applications of colorimetric and chromatographic techniques (GC-MS, HPLC-MS) in analysis of pesticide residue. Introduction to EPA regulatory body. Practical applications and examples in analytical chemistry and research.

B) Forensic Analysis

08 hrs.

Special features of forensic analysis, sampling, sample storage, sample dissolution, classification of poisons, lethal dose, significance of LD-50 and LC-50. General discussion of poisons with special reference to mode of action of cyanide, organophosphate and snake venom. Estimation of poisonous materials such as lead, mercury and arsenic in biological samples. Practical applications and examples in analytical chemistry and research.

Reference Books:

- 1. F. J. Welcher: Standard methods of Chemical analysis, 6th Ed. Vol. I and II(D. Van Nostard Comp.)
- 2. M. Kolthoff: Treatise on Analytical Chemistry Vol. I & II
- 3. F. D. Snell: Encyclopedia of industrial Chemical Analysis Vol. 1 to 20 (John Wiley)
- 4. Riech: Outline of Industrial Chemistry.
- 5. K. H. Buchel: Chemistry of Pesticides (John Wiley)
- 6. Indian, Pharmacopoeia, British Pharmacopoeia and U. S. Pharmacopoeia.
- 7. V. M. Parikh: Absorption spectroscopy of organic molecules (Addision Wesley)
- 8. Willard, Merrite, Dean and Settle: Instrumental methods of analysis (CBS)
- 9. D. H. Williams and J. Fleming: Specroscopic methods in organic chemistry (Mc Graw Hill) Silverstein: Spectroscopic Identification of organic compounds (John Wiley)
- 10. Jackmann and Sternhill: Applications of NMR spectroscopy of organic Chemistry (Pergamon Press)
- 11. J. D. Roberts : Nuclear Magnetic Resonance (Mc Graw Hill)
- 12. K. Benjamin : Mass Spectrometry
- 13. Nichollas: Aids to the Analysis of foods and Drugs.
- 14. A. H. Beckett and J. B. Stanlake; Practical Pharmaceutical Chemistry Vol. I & II (CBS publishers)

Course Outcomes (COs):

- CO 1: Students will gain knowledge of the instruments used at the interface of Analytical-Organic chemistry useful for R&D and structural elucidation using UV-Visible, IR, 1H & 13C NMR, Mass spectrometry data and interpretation of the same.
- CO 2: Students will acquire knowledge about the drug, their classification, sources of impurities (chemical, atmospheric and microbial contamination) in pharmaceutical raw materials and analysis of the same.
- CO 3: Students will gain knowledge about the conventional and advanced analytical approaches for analysis of drug, vitamin, body fluids and clinical samples.
- CO 4: Students will have an idea of commonly used pesticides and their analysis and also about forensic science and forensic sample analysis.

ACH303: Electroanalytical Techniques in Chemical Analysis

UNIT-I: Voltammetry Techniques

Introduction, Principle, excitation signals in voltammetry, basic instrumentation based on operational amplifiers, voltammetric electrodes, modified electrodes. Hydrodynamic Voltammetry-Electrode profiles in stirred and unstirred solutions, Applications.

Cyclic Voltammetry: Instrumentation, Determination of analytes using cyclic voltammetry, Applications.

Pulse voltammetry: Introduction, Normal Pulse Voltammetry, Reverse pulse voltammetry, Differential pulse voltammetry, Square wave voltammetry.

Stripping voltammetry: Cathodic and Anodic stripping voltammetry, Electrodeposition step, Voltametric completion of the analysis, adsorptive striping methods.

Voltammetry with microelectrodes. Practical applications in analytical chemistry and research.

UNIT- II: Coulometry

Introduction: Theory and instrumentation, current-voltage relationship, controlled potential Coulometry, types of coulometric methods, coulometric titration, and applications. Practical applications in analytical chemistry and research.

UNIT –III: Particle Size Analysis

Introduction, Low angle LASER light scattering: Instrumentation, theoretical models, Mie

15 hrs.

15 hrs.

theory, Fraunhofer diffraction theory, particle size distribution analysis, Applications. Dynamic Light Scattering: Introduction, Instrumentation, photodetector sample cell and sample handling, Applications, Photosedimentation: Setting velocity and particle size, Stokes equation, Instrumentation, sedimentation modes, Particle size distribution analysis, photometric measurements and applications. Comparison with particle size measurements using XRD, SEM and TEM. Practical applications in analytical chemistry and research.

UNIT -IV: A) Ion selective electrodes

10 hrs.

Terminology, types and construction of electrodes, glass electrode, solid state and precipitate electrodes, liquid – liquid membrane electrodes, enzyme and gas electrodes, and applications.

B) Electrophoresis

05 hrs.

Introduction: paper electrophoresis: Technique, factors affecting migration of ions, capillary and zone electrophoresis and applications. Practical applications in analytical chemistry and research

Reference Books:

- 1. R.D. Braun, Introduction to Instrumental Analysis.
- 2. D.A.Skoog, F. J. Holler, Principles of Instrumental Analysis, 6th edition.
- 3. Willard, Deritt, Dean and Settle, Instrumental methods of Analysis.
- 4. F. J. Welcher, Standard Methods of chemical Analysis Vol.3, PartA & B.
- 5. G.W. Ewing, Instrumental Methods of Analysis 4th and 5th editions.
- 6. Chatawal and Anand, Instrumental Methods of Analysis.
- 7. Bassett, Denney-Jeffer and Mendham, Vogel's Textbook of Quantitative Inorganic Analysis, (5th edition).
- 8. Electro-analytical chemistry, edited by H.W. Nurnberg.
- 9. Stulic, Ion selective electrodes (John Wiley).

Course Outcomes (COs):

- CO1: Fundamental knowledge of electrochemistry, electrodes, types of electrodes, its construction will lay foundation for the course.
- CO2: Students will gain knowledge and skill in electroanalytical techniques like cyclic voltammetry and its types, polarography, coulometry and dynamic light scattering technique for qualitative and quantitative analysis.

- CO3: Students will be familiar with the advanced electrodes used for chemical analysis, liquid-liquid membrane electrodes, enzymes and gas electrodes.
- CO4: Students will learn about electrophoretic techniques, advances in electrophoresis techniques and its analytical applications.

PR-ACH305: Analytical Chemistry Practical (2 Cr) 60 hrs.

Major Experiments:

- 1. Estimation of Sn, Cu and Pb from Bronze/Brass alloy (volumetric, gravimetric or colorimetric techniques can be used)
- 2. Analysis of Galena ore
- 3. Analysis of Benzoic acid and salicylic acid from medicated powder
- 4. Estimation of Aspirin
- 5. Determination of pK value of an indicator.
- 6. Cement analysis
- 7. Analysis of bauxite ore to estimate the amount of silica, aluminium and iron.
- 8. Estimation of salicylic acid and zinc oxide from medicated powder
- 9. Determination of saponification value and iodine value of oil
- To determine stability constant of Ferric ammonium sulphate and sulphosalicylic acid by Jobs variation method
- Studies on effect of substituent at orthoposition of benzoic acid on it's equilibrium constant pH-metrically
- 12. Simultaneous spectrophotometric determination of Cr and Mn.
- 13. Analysis of milk.

Minor Experiments:

- 1. Analysis of plaster of Paris for calcium content.
- 2. Estimation of copper fungicide.
- 3. Analysis of sulpha drug.
- 4. Analysis of vitamin-C in juices and squashes.
- 5. Analysis of ethambutol.
- 6. Identification of organic compounds by their IR spectra.

- 7. Determination of strength of acetic acid in commercial vinegar by conductometric method.
- 8. Determination of chloride content from saline water by potentiometry.
- 9. Estimation of bicarbonate and carbonate by potentiometric method.
- 10. Determination of pK of given dibasic acid pH-metrically.
- 11. Determination of pK of given dibasic acid potentiometrically.
- 12. Estimation of Fe from soil sample.
- 13. Analysis of Na and K from soil sample.
- 14. To estimate the amount of barium from given water sample by nephelometry.
- To determine the ion exchange capacity of active group of given cation exchange resin.
- 16. Estimation of lactose from milk sample using flame photometer.
- 17. To determine the amount of alkali content of antacid tablet titrimetrically.
- 18. Determination of pK value of tribasic acid, by potentiometry.
- Estimation of acetyl salicylic acid in the given aspirin tablet by titrating against 0.1N alcoholic KOH potentiometrically.
- 20. To determine the acid base dissociation constant and isoelectric point of amino acid pH metrically

Course Outcomes (COs):

- CO1: The students will acquire hands on training for conducting the representative experiments for the analysis of wide variety of samples of inorganic, organic and physical approaches by qualitative and quantitative analysis
- CO2: Student would learn the sample preparation and characterization for purity and qualitative and quantitative analysis of samples.
- CO3: Students will have good experimental skills for separation and estimation of amount of metal, metal ions in given samples.
- CO4: Students will be acquainted with the separation and estimation of organic compounds in given samples.

NOTE: Student should perform their practical work in the laboratory minimum 15 days in one semester for 2 credits.

RP-ACH306, Research Project (4 Cr, 120 Hrs)

See Annexture-I for details.

M. Sc. II (Sem - IV) Analytical Chemistry

ACH401: Modern Separation Methods in Analysis

UNIT-I: Advanced Gas Chromatographic Techniques

Principles, Plate theory, Instrumentation and working of a Gas Chromatograph, sampling, sample pretreatment, sample injection types, columns, Detectors, programmed temperature G.C., Applications. Gas chromatography-Mass Spectrometry, interface, instrumentation and applications. Practical applications and examples in analytical chemistry and research.

UNIT-II: Advanced Liquid Chromatographic Techniques

High Performance Liquid Chromatography (HPLC) and Ultra Performance Liquid Chromatography (UPLC)-Principle, instrumentation, mobile phase, Stationary support in HPLC, detectors and applications. Super critical fluid chromatography (SCFC), characteristics, instrumentation and applications. Comparison of HPLC and GLC with SCFC. Liquid Chromatography-Mass Spectrometry interface, instrumentation, advantages and applications. Practical applications and examples in analytical chemistry and research.

UNIT-III: Ion Chromatography

Principles, structure and characteristics of resins, eluent, supressor columns and detectors used in Ion Chromatography, commercial scope, analytical applications, environmental speciation by Ion Chromatography. Practical applications and examples in analytical chemistry and research.

UNIT –IV: A) Modern extraction and separation techniques 08 hrs.

Basic principles, classification of solvents extraction systems, extraction equilibria, factors affecting extraction process, application of β - diketones, δ Hydroxyquinoline, dithicarbamaes, xanthenes, Thio, separation of nonmetals and metals. Separation of transition metal ions using ion exchangers.

B) Extractive Chromatographic Separations

Introduction, Theoretical aspects of extraction chromatography, extraction chromatography with chelating ligands, extraction chromatography by ion pair formation, extraction

15 hrs.

15 hrs.

15 hrs.

chromatography by solvation, extraction equilibria, nature of stationary phase in extraction chromatography, inert support, techniques in extraction chromatography, extraction chromatography with tributyl phosphate and other applications. Practical applications and examples in analytical chemistry and research.

Reference Books:

- 1. A.I. Vogel, a text Book of Quantitative Inorganic Analysis.
- 2. W H Willard, L L Merritt and J A Dean, Instrumental Methods of Analysis.
- 3. S. M. Khopkar, Basic Concepts in Analytical Chemistry.
- 4. LR. Shyder and C.H. Harvath, An Introduction to separation Science. Wiley Interscience.
- 5. James S Fritz and George H.Schenk Jr. Quantitative Analytical Chemistry, 2nd editions Allyn and Bacon Inc. Bosten.
- 6. J.G.Dick, Analytical Chemistry.
- 7. R.L.Pescok and L.D.Shield, Modern Methods of Chemical Analysis.
- 8. O.Samuelson : Ion Exchange separation in analytical chemistry (Jhonwiley, 1963)
- Y. Marcus and A. S. Kertes: Ion Exchange and solvent Extraction of metal complexes (Wiley – Interscience, 1969)
- J. A. Marinsky and Y. Marcus: Ion exchange and solvent Extraction (Marcel Dekker, INC , New York, 1973)
- G. H. Morrison and H, Freiser: Solvent Extraction in Analytical Chemistry (John Wiley, New York, 1958)
- 12. A. K. Da, S. M. Khopkar and R. A. chalmers: solvents Extraction of metals (Von Nostrant Ravinhold, 1970).

Course Outcomes (COs):

- CO 1: Students will learn about modern separation and chromatographic used for analysis of different type of samples
- CO 2: The student will understand instrumentation and mechanism of various separation techniques.
- CO 3: Student will acquire knowledge regarding various choice of instrument and detectors to be used for analysis depending on the sample and matrix.

CO 4: Student will learn fundamentals of extractive chromatography, types of extraction techniques, advances in extraction methods and their hyphenations with chromatography leading to addressing challenging problems in analytical chemistry.

ACH402: Organic Industrial Analysis

UNIT – I: Industrial Analysis

A) Analysis of oils, fats and Soaps

Introduction to natural fats and oils; isolation of oils from natural resources and their purification. Analysis of oils and fats: Softening point, Congeal point, Titre point, Cloud point, Iodine, saponification, acid, hyroxyl, R-M and Polenske value, Elaiden test, etc.

Introduction to soaps, manufacture of soaps (in brief), analysis of soaps: total anhydrous soap and combined alkali, potassium, water, free fatty acids, saponifiable and non-saponifiable matter in soaps, estimation of phenol, copper and germicidal agents in soaps, determination of inorganic fillers and soap builders, and other additives, estimation of soap in detergents (THAM method)

B) Analysis of Detergents

Classification of detergents, analysis of raw materials, separation as alcohol soluble and alcohol insoluble matter, additives in detergent formulation (chlorides, sulfates, phosphates, silicates, borates, oxygen releasing substances, CMC, EDTA, etc.), their role and analysis; analysis of active ingredients in detergents (methylene blue and Hyamine-1622 method).

UNIT – II: Food and Food Additive Analysis

A) Food Analysis

Food flavors, food colors, food preservatives, analysis of milk and milk products, adulterants in milk and their identification, analysis of honey, jam and their major component. Practical applications and examples in analytical chemistry and research.

B) Food Additive Analysis

Additives in animal food stuff: Antibiotics: penicillin, chlorotetracyclin, oxytetracyclin in diet supplements; Identification and estimation of growth promoting drugs such as. sulfaquinoxaline, methyl benzoquate, sulfanitran, pyrimethamine, nitrovin, nitrofurazone, acinitrazole, etc

07 hrs.

07 hrs.

08 hrs.
UNIT-III: Analysis of cosmetics products

Introduction to cosmetics, definition, types of cosmetics, background, development in cosmetic industry, issues in cosmetic industries (contamination and adulteration), future scope and role of analytical chemistry.

A) Analysis of cream and lotions

Composition of creams and lotions, determination of water, propylene glycol, non-volatile matter and ash content; estimation of borates, carbonates, sulphates, phosphates, chlorides, ammonia, nitromethane, oxalic acid, 4- hydroxy benzoic acid, sodium iodate, free formaldehyde, H₂O₂, mercatoacetic acid, titanium and zinc oxides. Practical applications and examples in analytical chemistry and research.

B) Analysis of face powder

Composition of face powder, estimation of boric acid, Mg, Ca, Zn, Fe, Al and Ba. Analysis of deodorants and antiperspirants-composition, analysis of fats and fatty acids, boric acid, magnesium, calcium, zinc, iron, titanium, aluminium, phenol, methanamine, hexachlorophenone, sulphonates, urea, etc. Practical applications and examples in analytical chemistry and research.

UNIT-IV: Analysis of Paints, pigments and petroleum products

A) Analysis of Paints and pigments

Composition of paint, preliminary inspection of sample, test on the total coating, separation and estimation of pigments, binder and thinner of latex paints; modification of binder, flash point of paints. Practical applications and examples in analytical chemistry and research.

(B) Analysis of petroleum products

Introduction, constituents and petroleum fractionation, quality control; - specific gravity, viscosity, cloud point, pour point, flash point, vapor pressure, Doctor test, sulphuric acid absorption, aniline point, and colour determination. Determination of water, neutralization value (acid and base numbers), ash content, sulphur and mercaptan sulphur. Determination of lead in petroleum; Analysis of coal and coke: Types, composition, preparation of sample, proximate and ultimate analysis calorific value by Bomb Colorimetry.

Reference Books:

- 1. S. R. Junk and H. M. Pancoast: Hand book of sugars(AVI)
- 2. B. Bilot and B. V. Well: Perfumary technology (JW)
- 3. I. M. Kolthoff: Treatise on Analytical Chemistry Vol. I and II
- 4. D. Pearson: Laboratory techniques in food analysis.

07 hrs.

08 hrs.

15 hrs.

08 hrs.

- 5. S. Ranganna: Handbook of Analysis and Quality control for fruits and vegetable products, 2nd Ed.(Mc Graw Hill.)
- 6. Nicholls: Aids to the analysis of foods and drugs.
- 7. G. J. Mountrey: Poultry product technology (AVI)
- 8. Karamer Twig: Quality control for food industry (AVI)
- 9. G. F. Longonan: the analysis of detergents and detergent products (JW)
- 10. A. Davidsohn & B. M. Mlwidaky : Synthetic detergents (Book center, Mumbai)
- 11. M. Ash and L. Ash: A formulary of cosmetic preparations. (G. Goodwin)
- Kurl Bauer, Dorothea Garhe, Horst Surburg: Common fregrance and flavour materials, (VCH publisher, New York)
- 13. F. J. Welcher: Standard Methods of Chemical analysis Vol I & II (6th Ed.)
- 14. S. N. Mahendru: Analysis of food products (Swan Publishers)

Course Outcomes (COs):

CO1: Acquire knowledge of handling and investigating the characteristics of the oils, fats, detergents and soap samples and analysis of the same providing opportunity in cosmetic, pharmaceuticals, dyes and polymers industries.

CO2: Student will gain knowledge and importance of food quality, probe for food adulteration and adulterants, food preservative, food flavors and analysis of their components.

CO3: Students will also gain knowledge about the animal food stuff and the additives added in the animal food stuff as antibiotics, dietary supplements and growth promoting drugs, preservatives etc. and analysis of the same.

CO4: Student will learn about the analysis of cosmetics, face powder, hair dyes and hair care products, types of cosmetics, precautionary measures and composition of the cosmetics and specific roles of the ingredients. Will acquire knowledge about the paints, pigments and petroleum products, composition and analysis of the same using conventional and instrumental techniques.

ACH403: Advanced Methods in Chemical Analysis

UNIT-I: Fluorescence and Phosphorescence Spectrophotometry

Fluorimetry, types of luminescence, Instrumentations, theories of fluorescence and phosphorescence, electronic transition, structural factors, solvatochromism, solvation dynamics, faith of excited molecules, solvent effect on fluorescence, effect of intermolecular process, fluorescence anisotropy and time domain fluorescence life time measurements. Relation between concentration with fluorescence and phosphorescence intensity, fluorescence quenching mechanism, resonance energy transfer. Chemiluminescence, Fluorescence sensing, Synchronous spectrum, Fluorescent nanomaterials. Practical applications, examples and problems in analytical chemistry and research.

UNIT-II: Kinetic Methods

Theoretical basis of kinetic methods of analysis, methods of determining amount of the substance, Tangent Method, Fixed Time and Concentration method. Addition Method, Oxidation Reactions of H_2O_2 with thiosulphate, iodide and amino, Enzyme catalyzed reactions. Inhibitors and Activators.

UNIT – III: Photoelectron spectroscopy

Basic principles, photoelectric effects, Photoionization process, Koopman's theorem, photoelectron spectra of simple molecules, ESCA, chemical shift, Auger electron spectroscopy – basic idea.

UNIT-IV: X-ray spectroscopy

Introduction, X-Ray generation, Properties of X-radiation, Interaction of X-Rays with matter, Instrumentation. X-Ray Absorption, X-ray Fluorescence, X ray Diffraction methods -Instrumentation and analytical applications.

Reference Books:

- 1. Gary D Christian, Analytical chemistry 6th edition. John Willey and sons INC (2003)
- 2. Kaur, Instrumental Methods of Chemical Analysis. Pragati Prakashan, Meerut.
- 3. W H Willard, L L Merritt and J A Dean, Instrumental Methods of Analysis.
- 4. S. M.Khopkar, Basic Concepts in Analytical Chemistry.
- 5. D. Skoog and D. West, Principle of Instrumental Analysis. Holl Seamlers.
- 6. E. Berlin, Principles and Practice of X-Ray Spectrometric Analysis, Plenum, New York.
- 7. J. Winefordner, S. Schulman and T O Haver: Luminescence Spectrometry in

15 hrs.

15 hrs.

15 hrs.

- 8. Analytical Chemistry. Wiely Interscience NewYork.
- 9. Gary D Christian, Analytical chemistry 6th edition. John Willey and sons INC (2003)
- 10. Engineering chemistry, R Gopalan, G. S. Nagrajan.
- 11. Engineering chemistry B. K. Sharma.

Course Outcomes (COs):

- CO1: Students will be skilled in the techniques like fluorescence, phosphorescence, types of quenching, FRET and applications of the same in Analytical Chemistry and for addressing research problems.
- CO2: Students will gain knowledge of the kinetic methods of analysis supporting the analysis and data procured in research.
- CO3: The students will acquire the knowledge of advanced method of chemical analysis XPS, XRF, fluorescence and phosphorescence spectroscopy which will be beneficial in research.
- CO4: Students will acquire knowledge of identifying types of plastic and will also be able to and determination of metallic impurities in plastics.

RP-ACH 405: Research Project (6 Credits)

See Annexture-I for details.

NOTE: Study tour is compulsory for M.Sc. Part- II Students to visit Chemical Industries in India.

Name of Program: M. Sc. Part II- APPLIED CHEMISTRY

The M.Sc. Applied Chemistry program offered by Shivaji University is a Two Years full time program. In order to make students more careers oriented and nurturing their scientific temperaments, students will get exposure to the depth of core understanding of various dimensions of Applied Chemistry during these two years the study.

1. Programme Outcomes (POs)

- PO1: Students will have a thorough knowledge in the fundamentals and application of modern chemical and scientific theories including those in all branches of Chemical sciences.
- PO2: Students will be able to design and carry out scientific experiments as well as accurately record and analyze the results of such experiments.
- PO3: Students will be able to use the evidence based comparative chemistry approach for organic, inorganic synthesis and analysis of the chemical compounds.
- PO4: Students will be skilled in problem solving, critical thinking and analytical reasoning as applied to scientific problems.
- PO5: Applied Chemistry Students will be able to clearly communicate the results of scientific task in oral and written formats. Students will be able to function as a member of an interdisciplinary problem solving team.
- PO6: Students will be able to explain the role of Applied Chemistry for addressing social, economic, and environmental problems.

2. Programme Specific Outcomes (PSOs)

- PSO1: This course will be able to get global level research opportunities to students to pursue Ph.D. programme, targeted approach of competitive exams such as, CSIR –NET/GATE/SET, Personality Development Programs, discipline specific competitive exams conducted by service commission, etc.
- PSO2: The students will be able to get employment opportunities in various chemical pharmaceutical, paint and dye industries.
- PSO3: Understands the background of Inorganic reaction and organic reaction mechanisms and instrumental methods of chemical analysis, separation techniques and analytical methods of general purpose.
- PSO4: To gains complete knowledge about all fundamental aspects Inorganic, Organic, Physical and Analytical Chemistry.

3. Framework of NEP 2.0 as per NEP-2020 for M. Sc. Degree in Applied Chemistry

Class	SEM	Level	Mandatory Subjects	Elective (Choose any one)	RM (4 Cr)	OJT/FP (4 Cr)	RP	Cumm.	Degree
М. Sc. П	ш	6.5	APCH301(4 Cr) APCH302(4 Cr) APCH303(4 Cr) PR-APCH305(2 Cr)	E-ICH 304(4 Cr) OR E-OCH 304(4 Cr) OR E-PCH-304(4 Cr) OR E-ACH 304(4 Cr) OR			RP- APCH306 (4 Cr)	22	M. Sc. Degree in Applied Chemistry
	IV	6.5	APCH401(4 Cr) APCH402(4 Cr) APCH403(4 Cr)	E-ICH 404(4 Cr) OR E-OCH 404(4 Cr) OR E-PCH 404(4 Cr) OR E-ACH 404(4 Cr) OR			RP- APCH405 (6 Cr)	22	After 3/4 yr. UG
Cumm. Cr for 1 Year PG Degree		for 1 gree	26 Cr	8 Cr			10 Cr	44 Cr	

4. Course Structure: M.Sc. II Applied Chemistry

Semester III

Major Mandatory

Course Code	Course Title	Credits
APCH301	Applied Inorganic Chemistry–I	4
APCH302	Applied Organic Chemistry–I	4
APCH303	Applied Physical Chemistry	4
PR-APCH305	Physical Chemistry Practical-V	2
RP-APCH306	Research Project	4

Major Elective (Choose any one)

Course Code	Course Title	Credits
E-ICH304	Organometallic and Bioinorganic Chemistry	4
E-OCH304	Drug and Heterocycles	4
E-PCH304	Solid State Chemistry	4
E-ACH304	Environmental Chemical Analysis and Control	4

Semester IV

Major Mandatory

Course Code	Course Title	Credits
APCH401	Applied Inorganic Chemistry–II	4
APCH402	Applied Organic Chemistry–II	4
APCH403	Advanced Organic Chemistry–II	4
RP-APCH405	Research Project	6

Major Elective (Choose any one)

Course Code	Course Title	Credits
E-ICH404	Energy and Environmental Chemistry	4
E-OCH404	Applied Organic Chemistry	4
E-PCH404	Surface Chemistry	4
E-ACH404	Applied Analytical Chemistry	4

5. Detailed Syllabus

M.Sc. Part-II (Sem- III) Applied Chemistry APCH 301: Applied Inorganic Chemistry – I

UNIT I: Electronic Properties of Transition Metal Complexes

15 hrs.

Energy terms, states, microstates, splitting of terms in weak octahedral and weak tetrahedral ligand field, spin selection rule, Laporte selection rule, relaxation of selection rule, band intensities and band widths, Orgel diagrams of dⁿ- configurations in octahedral and tetrahedral environments, Tanabe-Sugano diagrams(d² and d³configuration), calculation of Dq, B and β values, adjusted crystal field theory, MO diagrams for octahedral and tetrahedral complexes (with and without π -bonding), charge-transfer spectra, spectral properties of lanthanides and actinides.

UNIT II: Magnetic Properties of Transition Metal Complexes 15 hrs.

Origin of magnetism, types of magnetic behavior, energy terms, splitting of terms in weak octahedral and weak tetrahedral ligand field, magnetic behavior of transition metal complexes: valence bond approach and crystal field approach, quenching of orbital angular momentum, temperature-dependent magnetism, measurement of magnetic susceptibility using Gouy and Faraday methods, magnetic properties of lanthanides and actinides.

UNIT III: Reaction of Transition Metal Complexes

Labile and inert complexes, ligand substitution reactions: nucleophilic substitution (S_N 1 and S_N 2, dissociative and associative mechanism), electron transfer reactions (redox reactions): outer sphere and inner sphere mechanism, two electron transfers mechanism, reactions of coordinated ligands, isomerization reactions: isomerization involving geometrical isomers.

UNIT IV: Nanoscience and Nanotechnology

Introduction to nanoscience and nanomaterials and emergence of nanotechnology; Moore's law, classification of nanomaterials, 1D, 2D, 3D with their examples, experimental methods for preparation of nanomaterials: chemical and physical, synthesis of nanoparticles of gold, rhodium, silica, palladium, platinum, and silver; size dependent properties of nanoparticles: optical properties, M.P., surface to volume ratio, carbon: fullerenes and nanotubes, applications of nanotechnology and nanomaterials: nanobiotechnology, nanosensors, nanomedicines (drug delivery and diagnosis), nanophotonics, environmental remediation etc., implications of nanotechnology.

Reference Books:

- 1. Cotton and Willkinsons Advanced Inorganic Chemistry
- 2. J. D. Lee Concise Inorganic Chemistry
- 3. Puri, Sharma and Kalia Principles of Inorganic Chemistry
- 4. R. Gopalan and V. Ramalingam Concise Coordination Chemistry
- 5. Asim K. Das and Madhu Das Fundamental Concepts of Inorganic Chemistry, (Vol.5)
- 6. G. S. Manku- Theoretical Principles of Inorganic Chemistry
- 7. Datta and Shymal Elements of Magnetochemistry
- 8. Alen Sharp Inorganic Chemistry
- 9. Sulbha Kulkarni- Nanotechnology: Principles and Practice
- 10. J. Schulte Nanotechnology: Global Strategies, Industry Trends and Applications

Course Outcomes (COs):

- CO1 To understand basic facts and concepts in Electronic and Magnetic Properties of Transition Metal Complexes and its applications.
- CO2 To be familiarized with the emerging areas of emergence of nanotechnology and their applications in Applied Inorganic Chemistry.
- CO3 To understand basic concepts and its classifications in Nanotechnologies used in Applied Inorganic Chemistry.

15 hrs.

- CO4 Student will be able to understand the theory of transition metal Complexes and nanotechnology.
- CO5 Learners Gain complete knowledge about the Labile and inert complexes, ligand substitution reactions and reaction mechanism of transition metal complexes.
- CO6 Students will able able to understand the applications of nanotechnology and nanomaterials such as, nanobiotechnology, nanosensors, nanomedicines (drug delivery and diagnosis), nanophotonics, environmental remediation etc., and implications of nanotechnology.

APCH 302: Applied Organic Chemistry – I

Unit I: Molecular Orbital Theory

Introduction, aromaticity in benzonoids, alternant and non-alternant hydrocarbon, Huckels rule, energy level of pi molecular orbital and the concept of aromaticity, calculation of energies of orbitals in cyclic and acyclic systems and the stabilities of different systems. Calculation of charge densities, 'PMO' theory and reactivity index.

Unit II: Organic Synthesis

Wolff rearrangement, Sommelet-Hauser rearrangement, Stevens's rearrangement, Smiles rearrangement, Robinson ring annulations reaction, Simmon-Smith reaction, McMurry reaction, Heck reaction and Vilsmeier-Haack reaction.

Unit III: Organic Photochemistry

Introduction, photochemical processes. energy transfer, sensitization and quenching. singlet and triplet states and their reactivity, photoreaction of carbonyl compounds, enes, dienes, and arenes, Norrish reactions of acyclic ketones. Patterno-Buchi, Barton, photo-Fries and Di- Pi methane rearrangement reactions. photoreactions of vitamin-D. Photochemistry of vision and photosynthesis, singlet oxygen generation and reactions, applications of photoreactions and their applications for industrial synthesis.

Unit IV: Free radical reactions

Introduction, types of free radical reactions, detection by ESR, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridge-head, reactivity in attacking radicals, the effect of solvent on reactivity, allylic hydrogenation (NBS), oxidation of aldehydes to carboxylic

15 hrs.

15 hrs.

15 hrs.

acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salt, Sandmeyers reaction. Hunsdiecker reaction.

Reference Books:

- 1. J. March Advanced Organic Chemistry, Wiley
- 2. R. O. C. Norman and A. Coxon Modern Synthetic Reactions (Chapman and Hall)
- 3. M. B. Smith Organic synthesis (McGraw-Hill)
- 4. Clayden, Greeves, WarrenandWoothevs Organic Chemistry
- 5. R. K. Bansal Synthetic application in organic chemistry (Narosa)
- 6. Peter Sykes A Guide Book to Mechanism in Organic Chemistry (Orient-Longmans)
- 7. Benjomin R. Breslow Organic Reaction Mechanism
- 8. B. S. Gould Mechanism and Structure in Organic Chemistry
- 9. Hendrikson, Cram and Hammond Organic Chemistry
- 10. J. D. Roberts and M. C. Caeserio Basic Principles of Organic Chemistry
- 11. N. S. Issacs Reactive Intermediates in Organic Chemistry (J. Wiley)
- 12. R. K. Bansal Organic Reaction Mechanism (McGraw Hill)
- 13. K. K. Rohtgi-Mukherji Fundamentals of Photochemistry (Wiley-Eastern)
- 14. J. Kagan Organic Photochemistry (Academic press)
- 15. J. M. Coxon and B. Holton Organic photochemistry (Cambridge University Press)
- 16. A. Gilbert and J. Baggott Essentials of molecular Photochemistry (Blackwell Scientific publication)
- 17. N. J. Urro and W. A. Benjamin Molecular photochemistry
- 18. Cox and T. Camp Introductory photochemistry (McGraw-Hill)
- 19. R. P. Kundall and A. Gilbert Photochemistry (Thomson Nelson)
- 20. J. Coxon and B. Hallon- Organic Photochemistry (Cambridge University press)

Course Outcomes (COs):

- CO1 To impart the students a thorough knowledge about the mechanisms of several organic reactions of some selected functional groups in organic compounds.
- CO2 To understand concept of Applied organic chemistry in various spheres of chemical sciences.
- CO3 To give an elementary idea of organic reactions, molecular orbital theory, free radical reactions and organic synthesis in Applied Organic Chemistry.
- CO4 Students would acquire the knowledge about the Various types of Organic reactions.

- CO5 To understand concept of concept of aromaticity, PMO theory in details and ESR detections.
- CO6 Detail information about concept of free radical substitution mechanism at an aromatic substrate and neighboring group assistance in Applied Organic Chemistry topics.

APCH 303: Applied Physical Chemistry

Unit I: Equilibrium Properties of Electrolytes

Non-ideal behavior of electrolyte solutions, Debye – Huckeltheory of inter-ionic attraction, ionic atmosphere, time of relaxation, relaxation and electrophoretic effects, Debye – Huckel-Onsagar equation, validity of Debye – Huckel equation, Debye – Falkenhagen effect, Wein effect, Debye - Huckel limiting law equation, ionic mobility, determination of dissociation constant by EMF method, experimental determination of ionic mobility, osmotic coefficient, Bjerrum theory, association constant, numerical problems.

Unit II: Catalysis: Principles and Applications

Basic principles of catalysis, adsorption isotherms, surface area pore size and acid strength measurement (TPD, pyridine IR acid base titration), Enthalpy and entropy of adsorption, interpretation of chemisorptions based on the structure and the nature of the solid – solid state theories – role of defects in catalysis, selection, preparation and evaluation of catalysts – test reaction, promoters, carriers and stabilizers, mechanism of selected reactions, hydrogenation and dehydrogenation reaction– dehydration of alcohols, olefin hydrogenation, decomposition of nitrous oxide, oxidation of CO- etonization of carboxylic acids, cracking of hydrocarbons.

UNIT III: Fuel cell and Corrosion

Fuel cell: Introduction, types of fuel cell, Hydrogen – oxygen fuel cells, hydrocarbon - air fuel cell, alkaline fuel cells, phosphoric acid fuel cell (PAFC), proton exchange membrane fuel cells (PEMFC), solid oxide fuel cells, molten carbonate fuel cell (MCFC), solid polymer fuel cell (SPFC), applications of fuel cell.

Corrosion: Introduction, theories of corrosion, comparison between dry and wet corrosion, factors affecting corrosion, prevention of corrosion, corrosion inhibitors, types of corrosion, passivity.

15 hrs.

15 hrs.

Unit IV: Nanomaterials

Introduction, Preparations and applications of nanomaterials-Synthesis of nano materials via –gas phase and liquid phase methods, high energy ball milling metal-semiconductorceramics and composites- size dependent properties - uniqueness in these properties compared to bulk and microscopic solids– nanomaterials and nanostructures in nature, TiO₂, ZnO, ZrO₂, Composites and their applications.

Reference Books:

- 1. G.W. Castellan Physical Chemistry (Addision-Lesley Publishing Co.)
- 2. E. A. Moelwyn Hughes Physical Chemistry (Pergamon Press)
- 3. L. C. Chapoy Recent Advances in Liquid CrystallinePolymers
- 4. D. R. Crow The Principles of Electrochemistry -(Chapman and Hall)
- 5. J.O.M.Bokris and A.K.N. Reddy Modern Electrochemistry (Plenum Rosatta)
- 6. A. W. Adamson Physical Chemistry of Surfaces
- 7. D. J. Shaw Introduction to Colloid and Surface Chemistry
- 8. J. J. Bikermann Surface Chemistry
- 9. Gurdeep Raj Advanced Physical Chemistry (Goel Publishing House, Krishna Prakashan Media (P)Ltd., Meerut
- 10. Pahari S. Physical Chemistry (New Central Book Agency (P) Ltd.) Kolkata
- J.N. Gurtu and A. Gurtu Advanced Physical Chemistry, 11th Edition (Pragati Prakashan)
- 12. D. N.Bajpai Advanced Physical Chemistry (S.Chand Publications)
- Arun Bahl, B S Bahl, G D Tuli Essentials of Physical Chemistry (S Chand Publication)
- 14.S H Maron and C F Prutton -Principles of Physical Chemistry
- 15. B. Viswanathan, S. Sivasanker and A. V. Ramaswamy Catalysis: Principles and Applications.
- 16. Introduction to Nanoscience and Nanotechnology, Gabor.L et al

Course Outcomes (COs):

CO1 This paper will provide an insight into some of the fundamental concepts in Equilibrium Properties of Electrolytes specifically Debye – Huckel Onsagar equation, Bjerrum Theory, Debye – Falkenhagen effect, Wein effect.

- CO2 To get an overview of principle and applications of catalysis and mechanism of selected reactions such as, hydrogenation, dehydrogenation olefin hydrogenation etc.
- CO3 To understand the principle and applications of fuel cell and corrosion.
- CO4 Students will be able to analyze and simulate the performance of different type of fuel cells.
- CO5 Students will be able to understand the basics of corrosion & apply their knowledge for protection of different metals from corrosion.
- CO6 Students would acquire the knowledge about basic understanding concepts of Applied Physical Chemistry concepts.

PR-APCH305: Applied Chemistry Practicals (2 Cr.) 60 hrs.

- 1. Preparation of coordination complexes (four)
- 2. Ion exchange study of separation of mixtures & estimations
- 3. Spectrophotometry
- 4. Nephelometry
- 5. Potentiometry
- 6. Conductometry
- 7. Determination of latent heat of fusion of a given solid.
- 8. Determination of stoichiometry and instability constant silver ammonia complex.
- 9. Determination of equivalent conductance at infinite dilution and dissociation constant for weak acid using Kolharausch Law of independent ionic mobility.
- 10. pH-metric determination of dissociation constant of carbonic acid.
- 11. To determine the dissociation constant of orthophoshoric acid by pH metrically.
- 12. Determination of order of reaction for iodination of acetone catalyzed by acid with reference to acetone, iodine and acid catalyst.
- 13. To determine stoichiometry and stability constant of ferric-salicylate complex by Job's Method and mole ratio method spectrophotometrically.
- 14. Preparation of m-nitroaniline
- 15. Preparation of Benzaanilide from benzophenone
- 16. Preparation of pthalimide
- 17. Preparation of N-bromosuccinimide
- 18. Preparation of 4-methyl-7-acetoxy coumarin
- 19. Preparation of 1,2,3,4-Tetrahydro carbazole

(Any other relevant experiments may be added if required)

NOTE: Student should perform their practical work in the laboratory minimum 15 days in one semester for 2 credits.

Reference Books:

- 1. A. I. Vogel, "A Textbook of Quantitative Inorganic Analysis", Longman
- 2. Gurudeep Raj, Advanced Practical Inorganic Chemistry, Krishna Prakashan.
- 3. W. G. Palmer, "Experimental Inorganic Chemistry", Cambridge University Press
- 4. J. B. Yadav, Advanced Practical Physical Chemistry, Krishna Publishers.
- 5. I. M. Kolthoff, V. J. Elving and Sandell, "Treatise on Analytical Chemistry", Interscience.
- 6. Instrumental Methods for Chemical Analysis-H. Kaur
- 7. Spectroscopy- B. K. Sharma
- 8. Instrumental Methods of Analysis-Willard, Merritt, Dean, Settle
- 9. Nanotechnology: Principles and Practices- Sulbha Kulkarni
- 10. Principles of Inorganic Chemistry-Puri, Sharma, Kalia
- 11. Concise Coordination Chemistry-R. Gopalan, V. Ramalingam
- 12. Elements of Magnetochemistry-Datta and Shymal
- 13. G.Zhong Cao. Nanostructures and Nanomaterials: Synthesis, Properties and Applications, Imperial College Press (2004).
- 14. T. Pradeep, Nano The Essentials: Understanding Nanoscience and Nanotechnology.
- 15. A Text Book of Quantitative Inorganic Analysis: A.I. Vogel.
- 16. Practical Physical Chemistry: B. Viswanathan and P.S. Raghavan, 2nd edition, (2012).
- 17. Systematic Experimental Physical Chemistry :S. W. Rajbhoj and T.K. Chondhekar.
- Experiments in Physical Chemistry by Carl Garland, Joseph Nibler, David Shoemaker 8th Edition, Kindle Edition.

Course Outcomes (COs):

- CO1 Students will get ability in professional sampling and sample treatment before actual analysis.
- CO2 Ability to treat and evaluate the results organic compounds and its purity.
- CO3 Understanding and capability of performing basic chemical processes and spectroscopic techniques in a chemical laboratory.

- CO4 Capability of performing measurements on basic analytical instruments (p^H meters, spectrometers, colorimeter, nephelometer, potentiometer, conductometer etc.)
- CO5 Students will get knowledge of safety signs on container of chemicals, handling of chemicals, and MSDS sheets.
- CO6 Students will have ability to synthesize commercial products and based on the experience of practical work, and to start their R & D laboratory.

RP-APCH306: Research Project

See Annexture-I for details.

M.Sc. Part-II (Sem- IV) Applied Chemistry

APCH401: Applied Inorganic Chemistry- II

Unit I: a) Infrared and Raman Spectroscopy

15 hrs.

15 hrs.

Molecular vibrations, force constants, diatomic model, simple harmonic oscillator, anharmonic oscillator, Raman spectroscopy, classical and quantum mechanical theory of Raman effect, use of symmetry considerations to determine the number of lines in IR and Raman Spectra: mutual exclusion rule, selectionrule in inorganic structure determinations: hydrogen bonding and infrared spectra, metal ligand and related vibrations, applications of Raman and Infrared spectroscopy.

b) Microwave spectroscopy

Basic concept, rotation spectra of simple inorganic compounds, classification of molecules, rigid rotor model, effect of isotopic substitution on transition frequencies& intensities non rigid rotor, stark effect nuclear and electron spin interaction and effect of external field. Applications of micro wave spectroscopy.

Unit II: Electron Spin Resonance Spectroscopy

Principle, fine, hyperfine, super-hyperfine and zero field splitting, ESR of d¹ and d⁹ transition metal ions; g values and factors affecting on g values, instrumentation and applications.
Mossbaur Spectroscopy: Introduction, Principles, Mossbaur nuclei, Mossbaur effect, Instrumentation, isomer shift, Quadrapole splitting and hyperfine interactions, applications.

Unit III: Spectroscopic & Microscopic Characterization techniques of Inorganic Materials 15 hrs.

Spectrometric techniques: UV-VIS-NIR spectroscopy, Energy dispersive X-ray spectroscopy (EDS), X-ray photoelectron spectroscopy (XPS)

Microscopic techniques: Transmission Electron Microscopy [TEM]; High resolution Transmission Microscopy [HRTEM]; Scanning Electron Microscopy [SEM];Scanning Tunneling Microscopy [STM]; Atomic Force Microscopy [AFM]

Unit IV: Instrumentation for Characterization of Inorganic Materials 15 hrs.

- a) X-ray Diffraction (XRD)
- b) Superconducting Quantum Interface (SQUID) Maganetometry
- c) Brunauer-Emmett-Teller Gas Absorption Surface Area Measurement and Pore Structure Analysis (BET Method)
- d) Dynamic light scattering (DLS)

Reference Books:

- 1. Instrumental Methods for Chemical Analysis-H. Kaur
- 2. Spectroscopy (Atomic and molecular)- Gurudeep R. Chatwal and Sham K. Anand
- 3. R. S. Drago, Physical Methods in Chemistry, Saunders College Publishers (1977).
- 4. Spectroscopy- B. K. Sharma
- 5. Instrumental Methods of Analysis-Willard, Merritt, Dean, Settle
- 6. Nanotechnology: Principles and Practices- Sulbha Kulkarni
- 7. K J Klabunde, Nanoscale materials in Chemistry, Wiley Interscience 2001
- 8. A R West, Basic Inorganic Chemistry, II Ed, Jhon Wiley & Sons (1999)
- 9. C. N. Benwell and E. M. McCash, Fundamentals of Molecular Spectroscopy, TataMcgraw Hill, New Delhi (2006).

Course Outcomes (COs):

- CO1 To understand the concept of Infrared and Raman Spectroscopy and its problems.
- CO2 This course will promote understanding about the microwave spectroscopy.
- CO3 Make Students aware of the fine structure of ESR absorption, Hyperfine structure, g values and factors affecting on g values, instrumentation and applications of ESR spectroscopy.
- CO4 Understand the principles and applications of Mossbauer spectroscopy.

- CO5 Also to understand some Spectroscopic & Microscopic Characterization techniques of Inorganic Materials such as TEM, HRTEM SEM, STM etc.
- CO6 Also to gain skill of various characterization techniques in material science for various research purposes.

APCH402: Applied Organic Chemistry – II

synthesis, structure of DNA. Structure of starch, cellulose Glycogen and Chitin.

Unit I: Chemistry of Biopolymers

Amino acids: Introduction and classification, protection and deprotection of N-terminus and C-terminus of amino acids, Peptides and their synthesis. Solid phase peptide synthesis (SPPS) Proteins: Structure and classification, Chemistry of nucleic acid bases A.G.C.T and U and their

Unit II: Pericyclic Reactions

Molecular orbital symmetry, Frontier orbitals of ethylene 1, 3butadiene, 1, 3, 5, hexatriene and allyl system, classification of pericyclic reactions, Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions – conrotatory and disrotatory motion, 4n, 4n+2 and allyl systems. Cycloadditions – antarafacial and suprafacialaddition, 4n and 4n+2 systems, 2+2 addition of ketens, 3, 3, dipolar cycloadditions. Sigmatropic rearrangements – Suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3, 3, and 5, 5 sigmatropic rearrangements. Ene reaction.

Unit III: Chemistry of Drugs & Pharmaceuticals

- A) Drugs: Classification of drugs based on activity. Synthetic procedure for the present commonly used dregs of each type, Manufacturing of few important drugs.
- **B)** Vitamins: Type of vitamins, synthetic of Vit A and Vit E, Vitamine II of niacinamide.

Unit IV: Heterocycles

Six membered Heterocycles with one heteroatom: Synthesis and reactions of pyrillium salts and pyrones and their comparison pyridinium and thiopyrylium salts and pyridines. Synthesis and reactions of coumarins, chromones.

Six membered heterocycles with two and more heterocycles: Synthesis and reactions of diazines and triazines. Seven membered heterocycles: Synthesis and reactions of azepines, oxepines and thiepines.

15 hrs.

15 hrs.

15 hrs.

Reference books:

- 1. Text book of polymer science, F. W. BillmeyersJr Wiley
- 2. Polymer science, V. R. Gowarikar, N. V. Vishwanathan and J Shreedhar, Wiley
- 3. Functional monomers and polymers, K. Takemote, Y. Inkiand R. M. Ottanbrite.
- 4. Contemporary polymer chemistry, H. R. Alcoek and F. W. Lambe, Practice Hall.
- 5. H. Arora, Organic Photochemistry and Pericyclic Reactions
- 6. Lendieer and Mitscher: The organic chemistry of drug synthesis (I. W.)
- 7. Burger Medicinal Chemistry.
- 8. A. Kar: Medicinal Chemistry.
- 9. W. O. Foye: Principles of Medicinal Chemistry.
- 10. R. M. Acheson : An introduction to chemistry of heterocyclic compounds (Interscience)
- 11. Joule and Smith: Heterocyclic Chemistry (Van Nostrand).
- 12. R. K. Bansal: Heterocyclic Chemistry (Wiley E).
- 13. L. A. Paquitte: Principles of Modern Heterocyclic Chemistry.
- 14. M. H. Palamer: The structure and reactions of heterocyclic compounds.
- 15. A. R. Katritzky: Advances in heterocyclic chemistry
- 16. Finar: Organic Chemistry (Vol. 1 & 2)
- 17. Cohn and Stumpt: Outline of Biochemistry.
- 18. Williams: Introduction to the chemistry of enzyme action.
- 19. The organic chemistry of drug design and drug action, R. B. Silverman Academic press.
- 20. Strategies for organic drug synthesis and design, D. Lednicer, J. Willey.

Course Outcomes (COs):

- CO1 Students will understand the concept building blocks of biomacromolecules.
- CO2 Students will have an idea regarding Classification, Structure and functions of different bioorganic molecules.
- CO3 The students will understand some fundamental aspects of applied organic chemistry.
- CO4 Student also will learn mechanism of some organic reactions, classification of pericyclic reactions.
- CO5 To aware the students about the knowledge of some organic drugs and its pharmaceutical applications.
- CO6 Students will have an idea regarding some important heterocyclic reactions and its mechanism.

APCH403: Advanced Organic Chemistry – II

Unit I: Aromaticity and some reaction

- A) Non benzenoid aromatic compounds: Aromaticity in Non- benzenoids compounds Annulenes and heteroannulenes, fullerenes, tropone, tropolone, azulene, fulvene, tropylium salts, ferrocene, three and five membered systems. Crown ether complexes, cyclodextrins, cryptands, catenanes and rotaxanes, bonding in fullerenes.
- **B)** Reaction mechanism: Alkyne metathesis reaction, Weinreb ketone synthesis, Petasis reaction, Henry reaction, Corey Kim oxidation. Reactions of carboxylic acids and esters.

Unit II: Kinetic and thermodynamic control of reactions 15 hrs.

Nitration and Sulphonation of naphthalene, Wittig reaction, Enolization, Friedel-Crafts and Diels Alder reactions.

Oxidation: Oxidation with Cr and Mn Compounds: oxidation of alcohol, aldehyde, C=C, C-H bonds in organic molecules, Pyridiniumchloro chromate (PCC), Oxidation with peracids and other peroxides: C=C, Sharplessepoxidation.

Other types: Prevost and Woodward hydroxylation, cis and trans-hydroxylation, glycol cleavage reagent. HIO₄, Pb(OAc)₄, mercuric acetate, SeO₂, DDQ.

Unit III: Chemistry of Natural Products

- **A) Terpenoids:** Structure and synthesis of alpha-Pinene, Camphor, Cadenine and Caryophyllene. Hofmann, Emde and von Braun degradation.
- **B)** Alkaloids: Structure elucidation of Papaverine, Quinine and Morphine. Synthesis of quinine and Papaverine. Structure and synthesis of beta-carotene, classification and structure of lipids and their biofunctions.
- **C) Prostaglandings:** Nomenclature, structure (not elucidation) and biosynthesis of Prostaglandins PGE₂, and PGF_{IV.}

Unit IV: Selected Organic Reactions and Reagents

Lithium dimethyl cuprate, Trimethylsilyl iodide, Baker Yeast, Phase-transfer catalysts. 1, 3dipolar cyclo addition and chelotropic reactions, sigmatropic rearrangement, supra and antarafacial shifts of H, Sigmatropic shifts involving carbon moieties, (3,3) and (5,5) sigmatropic rearrangement and Claisen and Cope and Aza Cope rearrangement, Ene reaction.

15 hrs.

15 hrs.

Reference Books:

- 1. L. M. Hardwood, Polar rearrangements, Oxford University
- 2. J. March, Advanced Organic Chemistry, Wiley
- 3. S. N. Issacs, Physical Organic Chemistry, Longman
- 4. P. Y. Bruice, Organic Chemistry, Prentice Hall
- 5. H. Arora, Organic photochemistry and Pericyclic reactions
- 6. C. H. Dupuoy, and O. L. Chapman, Molecular reactions and Photochemistry, Prentice Hall
- 7. J. M. Cozon and B. Holton, Organic Photochemistry, Cambridge University Press
- 8. S. H. Pine, Organic Chemistry by McGraw-Hill
- 9. I. L. Finar, Organic Chemistry Vol W, Longman

Course Outcomes (COs):

- CO1 To develop interest among students in advanced organic chemistry.
- CO2 To impart essential theoretical knowledge about aromaticity and some reactions.
- CO3 To aware about the idea and knowledge about Kinetic and thermodynamic control of reactions.
- CO4 To details study about the some oxidation reaction with Cr and Mn compounds and some other types.
- CO5 The students can apply their knowledge for synthesis of various natural products like n their research terpenoids, alkaloids and prostaglandings.
- CO6 Students will have an idea about selected organic reactions and reagents and some sigmatropic rearrangements.

RP-APCH405: Research Project

See Annexture-I for details.

NOTE: Study tour is compulsory for M.Sc. Part- II Students in Sem-IV to visit Chemical Industries in India.

Name of Program: M.Sc. Industrial Chemistry

The Indian chemical industries occupy a unique position in the Indian economy in terms of contribution to employment and export potential. In spite of a strong natural resourcebased India's share in the global market is major one. The experts in Industrial Chemistry have emphasized the need for capital infusion capacity, modernization and up gradation in various segments of industrial processes to bring about efficiencies and economies of scale in order to achieve in global markets. Keeping in view the need of Indian industries, Shivaji University has started M.Sc. course in Industrial Chemistry from academic year 1993-1994 in the Chemistry. Department to educate and train the science graduates in industrial chemistry to serve the industrial sector as a technical, R & D personnel and quality control production personnel to manage the industrial production and contribute to the development of nation.

One of the objectives of the M.Sc. Industrial Chemistry Course is to attain new heights in industrial teaching and research and to provide trained man power to vast developing Indian industries to develop the young graduate as a premier precision tool for future creation. M.Sc. course in industrial chemistry is a potential base provided by the Shivaji University on the University campus to educate the students from rural area who will get employment on large scale in Indian Chemical industries. Since last twelve years, M.Sc. industrial chemistry students have obtained employment on large scale in Indian chemical industries.

1. Course Structure: M.Sc. II, Industrial Chemistry <u>Semester- III</u>

No	Course	Mandatory	Title of the paper	Hours	Cr
	Code	/Elective			
1	INDCH301	Mandatory	Organic Chemical Industries-I	60	4
2	INDCH302	Mandatory	Inorganic Chemical Industries-I	60	4
3	INDCH303	Mandatory	Methods of Analysis in	60	4
			Industries		
4	E-ICH304	Elective	Organometallic and	60	4
			Bioinorganic Chemistry		
5	E-OCH304	Elective	Drug and Heterocycles	60	4
6	E-PCH304	Elective	Solid State Chemistry	60	4
7	E-ACH304	Elective	Environmental Chemical	60	4
			Analysis and Control		
5	PR-INDCH305	Mandatory	Industrial Chemistry Practicals	60	2
6	RP-INDCH306	RP	Research project	120	4

Semester- IV

No	Course	Mandatory/	Title of the paper	Hours	Cr
	Code	Elective			
1	INDCH401	Mandatory	Drug and Pharmaceuticals	60	4
2	INDCH402	Mandatory	Inorganic Chemical Industries-II	60	4
3	INDCH403	INDCH403 Mandatory Selected Topics		60	4
			Chemistry		
4	E-ICH404	Elective	Energy and Environmental Chemistry	60	4
5	E-OCH404	Elective	Applied Organic Chemistry	60	4
6	E-PCH404	Elective	Surface Chemistry	60	4
7	E-ACH404	Elective	Applied Analytical Chemistry	60	4
8	RP- INDCH405	RP	Research project	180	6

2. Program Outcomes (POs):

- 1. Industrial chemical processes are described and analyzed in terms of thermodynamic and kinetic aspects and are also highlighted the most important technology.
- 2. Industrial chemists make use of their broad understanding of chemistry and environmental sustainability in areas like pharmaceutical companies, polymer manufacturing, petrochemical processing, food science, and manufacturing industries.
- 3. Industrial chemists are constantly striving to improve the safety and efficiency of making important chemicals and materials.
- 4. **Process optimization** an industrial chemist plays a part in optimising production to produce large amounts of a substance
- Environmental monitoring and control industrial chemists work on the management and control of the environment during industrial processes, to ensure everything is being done to minimize the impact and work towards a clean and safe future.

3. Program Specific Outcomes (PSOs):

- Students should learn an advanced level understanding of at least three of the following areas of Chemistry - Analytical, Inorganic, Organic, and Physical Chemistry.
- 2. Students should broaden their professional foundations through activities such as teaching, internships, and project work.
- 3. Students should acquire the basic tools needed to carry out independent chemical research. Students should become proficient in their specialized area of chemistry and successfully complete an advanced research project.

4. Detailed Syllabus

M.Sc. Part-II (Sem- III) Industrial Chemistry

INDCH301: Organic Chemical Industries – I

Unit I: Dyes and Pigments

Dyes, Pigments and Intermediates: Classification of Dyes, Preparation of important dye intermediates, Methods of preparation of commercial dyes of different classes with suitable examples. Typical manufacturing processes of few dyes, fluorescent brightening agents, and Special dyes: Photosensitive dyes, dyes as food additives, natural dyes.

Unit II: Food Processing and food Additives

Classification, chemical composition and nutritional value of common food stuffs, properties of foods, food preservation and processing, food deterioration, methods of preservation and processing by heat, cold, chill storage, deep freezing, drying, concentration, fermentation, and radiation. Permitted food additives and their role; antioxidants, colouring agents, sweeteners.

Unit III: Cane Sugar Based Chemistry

Introduction, manufacturing processes of Acetic acid, oxalic acid, citric acid, acetic anhydride, furfural from bagasse, anhydrous alcohol, sugar based chemical industries in India. Preparation of organic jaggery, analysis of jaggery

Unit IV: Soap and Detergents

Oils, soaps and Detergents: Refining of edible oils, Manufacturing of soaps, Detergents, Liquid Soaps, aptholmic solution. Manufacturing of glycerol from fatty acids, greases from fatty acids, turkey – red oil.

Paints: Introduction, properties, manufacture of paint and applications **Varnishes and Inks:** Constitutions, examples of preparation and applications.

15 hrs.

15 hrs.

15 hrs.

Reference books:

- 1. K. Venkatraman: The Chemistry of Synthetic Dyes Vol. 1-7 (A.P)
- 2. Abranart: Dyes and Their intermediates (Pergaman)
- 3. Beech: Fiber reactive Dyes (Logos Press)
- 4. Frig and David Dyes intermediate
- 5. Allan: Color Chemistry
- 6. Kent: Riehels Industries Chemistry.
- 7. M Ash & I Ash: A formulary of paints & other coatings.
- 8. M Ash & I Ash: A formulary of cosmetic preparation (Godwin)
- 9. P.H. Groggings: Unit Processes in organic synthesis (MGH)
- 10. Kiik& other: Encyclopedia of Chemical technology.
- 11. L. W. Aurand, A. E. Woods, Food Chemistry, AVI Publishing Inc.
- 12. L. H. Mayer, Food Chemistry, Affiliated East-West Press Ltd., New Delhi.
- 13. N. Shakuntala Manay, M. Shadakhsara Swamy, Foods-Facts and Principles.
- 14. John M. deMan, Principles of Food Chemistry.
- 15. The Complete Book on Sugarcane Processing and By-Products of Molasses (with
- 16. Analysis of Sugar, Syrup and Molasses) -H. Panda

Course Outcomes:

Students will be able to

- CO1 Study the manufacturing process of dyes, pigments and intermediates
- **CO2** Gain basic idea regarding the food processing and importance of food additives in several industries
- **CO3** Learn the manufacturing of acetic acid, oxalic acid, citric acid, anhydrous alcohol from sugar cane molasses and its mechanism
- CO4 Usages of organic chemicals for the synthesis of various essential oils, soaps, detergents, paints and varnishes

INDCH302: Inorganic Chemical Industries – I

Unit I: Dairy and Leather Chemistry

A) Dairy Chemistry: Milk and milk products, composition and structure of milk, milk proteins, enzymes, vitamins, minerals, density and viscosity of milk, effect of heat on milk, milk processing, basic milk categories, butter, ghee and clarified butter.

B) Leather Chemistry: Introduction, constituents of animal skin, manufacture and preparation of hides, cleaning, soaking, limiting and degreasing, finishing and sharing, tanning; leather, vegetable, chrome, tanning effluents; pollution and control

Unit II: Cosmetics and Perfumes

A general study including preparation and uses of the following: Hair dye, hair spray, Shampoo, Sun- tan lotions, face powder, lipsticks, talcum powder, nail enamel, creams (cold, vanishing and shaving creams), antiperspirants and artificial flavours. Water: Special consideration for cosmetics use. Surfactants: Classification and application in cosmetics - Foaming agents, emulsifiers, and solubilizers. Classification and application in cosmetics Antioxidants, antimicrobial and chelating agents used as preservatives. Factors affecting effectiveness of antimicrobial preservatives

Unit III: Nanomaterials

Introduction, Preparations and applications of nanomaterials-Synthesis of nano materials via -gas phase and liquid phase methods, high energy ball milling metal-semiconductorceramics and composites- size dependent properties - uniqueness in these properties compared to bulk and microscopic solids- nanomaterials and nanostructures in nature, TiO₂, ZnO, ZrO₂, Composites and their applications.

Unit IV: Nanotechnology in Agriculture

Introduction, Precision farming, Smart delivery system - Nanofertilizers: Nanourea and mixed fertilizers, Nanofertigation - Nanopesticides, Nanoseed Science, organic manures, micronutrients, biopestiside, biofertilizers and agrochemicals.

15 hrs.

15 hrs.

15 hrs.

Reference books:

- 1. F A Henglein: Chemical Technology (pergamon)
- 2. R.W. Thomas and P. Farago: Industrial Chemistry (HEB)
- 3. E. Stocchi: Industrial Chemistry, Vol -I, Ellis Horwood Ltd. UK
- 4. P.C. Jain, M. Jain: Engineering Chemistry, Dhanpat Rai & Sons, Delhi
- 5. Introduction to Nanoscience and Nanotechnology, Gabor.L et al
- Fundamentals of Nanotechnology, Hornyak, G. Louis, Tibbals, H. F., Dutta, Joydeep, CRC Press, 2009
- 7. Nanomaterials: An introduction to synthesis, properties and application, Dieter Vollath, WILE-VCH, 2008
- 8. Lynn J. Frewer, WillehmNorde, R. H. Fischer and W. H. Kampers, Nanotechnology in the Agri- food sector, Wiley-VCH Verlag, (2011)
- 9. B.K. Sharma: Industrial Chemistry, Goel Publishing House, Meerut

Course Outcomes:

Students will be able to

- CO1 Know the different types of milk, milk products, and milk processing methods
- CO2 Get the essential knowledge of chemistry which they utilize in cosmetic and perfume industries
- CO3 Grab basic concept of nanomaterials and its potential applications in various industries
- CO4 Expose various emerging new area of nanoparticles synthesis and its various applications in agriculture and biofertilizers

INDCH303: Methods of Analysis in Industries

Unit I: Voltammetry Techniques

Introduction, Modified polarographic techniques, stationary electrode polarography, sinusoidal alternate current polarography, rapid scan polarography, pulse polarography, square wave polarography, Cyclic voltammetry, stripping voltammetry, numerical.

Unit II: NMR Spectroscopy

General introduction and definition; chemical shift; spin –spin interaction; shielding mechanism of measurement; chemical shift values and correlation for protons bonded to carbons [aliphatic; olefinic; aldehydic and aromatic] and other nuclei [alcohols; phenols; enols; acids; ammines; amides and mercapto]; chemical exchange; effect of deuteration; complex spin-spin interaction between two; three; four; and five nuclei [first order spectra]; virtual coupling. Stereochemistry; hindered rotation; Karplus curve variation of coupling constant with dihedral angle. Simplification, Simplification of complex spectra; nuclear magnetic double resonance; shift reagent; solvent effect. Fourier transform technique; nuclear overhauser effect [NOE] Resonance of other nuclei – F & P.

Unit III: Chemical Analysis of surfaces

Introduction to photoelectron spectroscopy, Ion Scattering Spectroscopy, Secondary Ion Mass Spectrometry, Auger Electron Spectroscopy, Electron Spectroscopy for Chemical Analysis. Basic principles, Instrumentation and applications of these techniques

Unit IV: Gas and Fuel analysis

Modern concept of fuels, classification of fuels, characteristics of good fuels, Orsat apparatus and its use in gas analysis, Instrumentation and working of bomb calorimetry, boy's calorimeter and numerical, coal analysis, calorific value of fuels, determination of calorific value of a solid or liquid fuel, Flash point, determination of flash point by Abel's method.

Reference books:

- 1. F. J. Welder: standard Methods of chemical analysis Voil. III Part A&B
- 2. H.A. Strobel chemical instrumentation (AW)
- 3. Willard, Merrit& Dean, Instrumental Methods of analysis (FWAP)
- 4. F.D. Snell, Encyclopedia of Industrial: Chemical Inorganic analysis Vol. 1 to 20 (J.W)

15 hrs.

15 hrs.

15 hrs.

- 5. Hillebrand, Lhundell and Hoffman: Applied inorganic analysis (Interscience)
- 6. D.K. Chakrabarty: Solid state Chemistry
- 7. H. Kaur, Instrumental method of analysis.
- 8. V.M. Parikh, Application spectroscopy of organic molecules. (Mehata)
- 9. D.W. Williams and Flemming, Spectroscopic methods of organic compound
- 10. Silverstein and Basallar, Spectroscopic identification of organic compounds
- 11. V. M. Parikh Absorption Spectroscopy for Organic Molecules (J. Wiley)
- 12. P.S. Kalsi Spectroscope of organic compounds (New age publisher)
- 13. Jackman and Sterneil, Application of NMR spectroscopy
- 14. J. D. Roberts, Nuclear magnetic resonance (J. Wiley)
- 15. D. L. Pavia, G. M. Lampman and G. S. Kriz, Introduction to Spectroscopy.
- 16. Analytical Chemistry- Gurudeep R. Chatwal Edited by Madhu Arora, Himalaya publication.

Course Outcomes:

Students will be able to

- CO1 Know the basic principles of different voltametric techniques employed for sample analysis
- **CO2** Investigate and determine the structure of typical organic chemical compounds using suitable nuclear magnetic resonance spectroscopy
- **CO3** Learn the theory behind surface chemical analysis using various tools, like XPS, ion scattering, secondary ion mass, Auger electron, and electron spectroscopy
- CO4 Get emerging techniques like Bomb, Boy's calorimeter for the analysis of various fuels

PR-INDCH305: Industrial Chemistry Practicals (2 Cr.)

A) Physical Chemistry Practicals

1. Conductometry

I] To determine the critical micelle concentration of sodiumlaurylsulphate in aqueous solution conductmetrically.

II] Determination of percentage of acetic acid in commercial vinegar solution

2. Fluorimetry

I] To estimate the Quinine sulphate in given sample by Fluorometry.

II] To determine the amount of riboflavin in given B-complex tablet.

3. Latent Heat of fusion

To determine the latent heat of fusion of given solid

4. Polarography

I] To study the effect of Oxygen supporting electrolyte and maximum suppressor and determine the half wave potential of Cd/Zn in given solution by Half wave potentialmethod. Differential method and half wave equation method.

II] To determine unknown concentrations of Cd^{+2} ion in given solution by standard addition method.

5. Potentiometry

I] To determine Solubility of PbI_2 with Ag/AgI electrode by using potentiometry.

II] To determine the dissociation constant of tri basic $acid(H_3PO_4)$ potentimetrically.

III] To determine the dissociation constant of dibasic acid by potentiometric method

6. pH metry

I] To determine the dissociation constant of dibasic acid pH – metrically.

II] To determine pH value of various buffer using pH meter and determination of dissociation constant of acetic acid.

III] To determine hydrolysis constant of aniline hydrochloride by pH metry.

IV] To determine isoelectronic point and dissociation constant of amino acid (Glycine) by pH metry.

7. Spectrophotometry:

I] To determine pK value of phenolphthalein indicator by spectrophotometric method.II] To study the stoichiometry and stability of ferric sulphate complex by Job's method and Mole ratio method.

III] To determine stability constant of Ferric thiocynate complex by Frank

Ostwald method spectrophotometrically

B) Organic Chemistry practical's

- 1. Identification and separation of ternary organic mixtures by physical and chemical methods.
- 2. Preparation of p amino benzoic acid from p toluidine (three step)
- 3. Preparation of p-iodonitrobenzene (three step)
- 4. Preparation of benzanilide from benzophenone by use of Beckmann's rearrangement (two step)
- 5. Preparation of m nitroaniline from nitrobenzene (two step)
- 6. Estimation of cu from copper fungicide
- 7. Estimation of Endosulfan
- 8. Estimation of Nitrogen by Kjeldahl's method

C) Inorganic Chemistry practical's

- 1. Ore Analysis -3
- 2. Alloy Analysis 3
- 3. Preparation of coordination complexes
- 4. Ion exchange study of separation of mixtures and estimations
- 5. Spectrophotometry
- 6. Separation and estimation of ions using ion exchange chromatography
- 7. Nephelometry
- 8. Potentiometry
- 9. Conductometry
- 10. Thermal analysis
- 11. Magnetic properties of transition metal complexes
- 12. Spectro Fluorimetry
- 13. Solvent extraction
- 14. Nuclear chemistry
- 15. Soil Analysis
- 16. Data analysi

(Any other relevant experiments may be added if required)

NOTE: Student should perform their practical work in the laboratory minimum 15 days in one semester for 2 credits.

Course Outcomes:

Students can be able to

- CO1 Learn how to use hazardous and non-hazardous chemicals and safety precautions and practical skills for analysing materials using modern analytical methods and instruments
- **CO2** Quantitatively preparation of organic compounds as well as their derivatives and estimation of various compounds
- CO3 Estimate various metal ions present in alloys by volumetric, colorimetric or gravimetric methods
- CO4 Handle various instruments such as conductometer, potentiometer, pH meter, spectrophotometer, and polarimeter

RP-INDCH306: Research Project

See Annexture-I for details.

M.Sc. Part-II Sem-IV

INDCH401: Drugs and Pharmaceuticals

Unit I: Drugs, Pharmaceuticals and Pharmaceuticals analysis 15 hrs.

Introduction & classification of the drugs based upon their mode of action, Q-SAR, Moleculardocking, Manufacturing processes of few important drugs, Aspirin, Ibuprofen, Paracetamoletc.

15 hrs.

Unit II: Drugs Acting on infectious diseases

Anthelmintic agents; synthesis of diethyl carbazine, niclosamide

Antitubercular drugs; synthesis of isoniazid, p-amino salicylic acid ethambutol and thioacetazone, Anti-leprosy drugs; synthesis of dapsone and clofazimine, Sulpha drugs; classification, mode of action, synthesis of sulfadiazine, sulphaisoxazole, sulfadimethoxine.

Unit III: Cancer therapy and Antineoplastic drugs

A) Cancer therapy: Types of cancers, Causes of cancer and therapy: surgery, radiation therapy, immunotherapy, chemotherapy, combination therapy, adjuvant therapy.

b) Antineoplastic drugs: Mercaptopurines,6-thioguanine, 5-flurouracil, allopurinol, methotrexate. Alkylating agents, effect of alkylating agents on DNA, DNA intercalating agents. Antimitotic agents and other therapeutic agents.

Unit– IV: Anti-AIDS, Cardiovascular and Anti-diabetic drugs 15 hrs.

A) Anti-AIDS: Introduction& mechanism of HIV multiplication, Pathogenicity of HIV diagnosis, ELISAtest, transmission and preventions of HIV, Anti-AIDS drugs

B) Cardiovascular drugs: Introduction, synthesis of amyl nitrate, methyldopa, sorbitrate.

C) Anti-diabetic drugs: Introduction, synthesis of sequence of A and B chain of insulin, Glibenclamide, metformin.

Reference books:

- 1. Burger: Medicinal Chemistry (I.W.)
- 2. W. O. Foye: Principle of Medicinal Chemistry (I.E)
- 3. Lendieer and Metscher: The Organic Chemistry of Drug Synthesis (I.W.)
- Essentials of Medicinal Chemistry; Editors Korolkovas and J. H. Burkhaltar, John Wiley & Sons
- 5. Wilson and Gisvold: Text Book of Organic Medicinal and Pharmaceutical Chemistry.
- 6. O. D. Tyagi: SyntheticDrugs.
- 7. Medicinal Chemistry G. R. Chatwal.
- 8. Principles of medicinal chemistry (4th edition) W.D. Foye, T.L. Lemke, and D. A. Williams.
- 9. Organic chemistry of drug action and design R. B. Siwerman
- 10. Synthetic Drug G. R. Chatwal.
- 11. Handbook of Industrial Chemicals (Vol.-I) K. M. Shah
- 12. Principles of Medicinal Chemistry Vol. I, S. S. Kadam and K.G.Bothara
- 13. A Text Book of Medicinal Chemistry P. Parimo

Course Outcomes:

Students will be able to

- CO1 Study the different kinds of drug synthesis, classifications and their applications in medicinal fields
- CO2 Explain how the anti-leprosy and sulpha drugs acts on infectious diseases
- CO3 Obtain the knowledge related to different types of cancers with causes of cancer and therapy on it
- CO4 Details mechanism of cancer therapy, antineoplastic drugs, anti-AIDS, cardiovascular and anti-diabetic drugs.

INDCH402: Inorganic Chemical Industries –II

Unit I: Metallurgy

15 hrs.

Metallurgy: Minerals in India, Mineral processing, Ellingham diagrams, manufacture and applications of metal alloys and salts, techniques for using low grade minerals. Iron and steel(Iron, Steel alloy, tool steel and stainless steel), Copper and its alloys, Zinc, Nickel and Aluminum.

Unit - II: Metal finish technology and Chloralkali Industries 15 hrs.

A) Metal finish technology: Electro refining of metals, electroplating of nickel, chromium, copper, cadmium, silver and Gold, surface treatment technology, surface coats. Introduction, Electrodeposition, electroplating (Factors affecting, requirements and applications), hot dipping, metal cladding, immersion plating, metal spraying, vapour deposition and chemicaland organic coating.

B) Chloralkali Industries: Soda Ash, Caustic Soda, Chlorine

Unit-III: Applications of Inorganic compounds in pharmaceutical chemistry 15 hrs. Applications of Inorganic compounds in pharmaceutical chemistry: Introduction, impurities in pharmaceutical substances and their limit test, antioxidants, gastrointestinal agents, topical agents, dental products, inhalants, expectorants, respiratory stimulants. Compounds of iron, iodine and calcium, antidotes in poisoning, pharmaceutical aids

Unit IV: Glass and Refractory materials, Industrial Gases and Chemicals of Utility 15 hrs.

A) Glass and Refractory materials: Raw materials, Soda glass, borosilicate glass, Lead Glass, Colored Glass, Refractory: Raw materials, clay pots, Zeolites.

B) Industrial Gases: Manufacture and industrial uses of H₂, O₂, N₂, CO₂ & acetylene. Liquefaction of gases, production of low temperatures,

C) Chemicals of Utility: Inorganic fine chemicals, magnesia, alumina, AlCl3, calcium carbonate, sodium silicate, MnO₂, FeSO₄, PbO₂, Na₂HPO₄ and NaOH.

Reference books:

- 1. Lowenheim F A (1974) Modern Electroplating III Ed Chapman & Hall, Landon.
- 2. Gable, D: Principal of metal Treatment and protection. Pergamon, Press Oxford (1978)
- 3. G.A. Keneth: Electroplating for Engineering's A Hand Book IIIrd EdnVan Nastrad Reinbold Co London
- 4. F A Lowinbein: Modern Electroplating, Electroplating Publication New Jersey
- 5. Burke Progess in ceramic science Vol. IV
- 6. R.R.Iash: afromulary of paints and other coating Vol. I
- 7. J.D. Gilchrist: Extraction Metallurgy (Pergamon)
- 8. W.H. Dennis: Foundation of steel and iron Metallurgy (Elsevier)
- 9. S.D. Shukla & G N Pandey: A text book of chemical technology Vol. 1
- 10. F A. Henglein: Chemical Technology (Pergamon)

Course Outcomes:

Students will be able to

- CO1 Understand the detail information of the processing and applications of several minerals
- CO2 Gain information about metal finishing technology, cladding, and products of chloralkli industries
- CO3 Pointed out various applications of inorganic compounds in pharmaceutical chemistry
- CO4 Explain manufacturing and industrial uses of H₂, O₂, N₂, CO₂& acetylene

INDCH403: Selected Topics in Industrial Chemistry

Unit I: Speciality polymers and preparation

Conducting polymers, Polyaniline, Polyacetylene, Polypyrrole, Polypropylene (PP), Polyvinyl chloride (PVC, PVDC & CPVC), Poly ethylene terphalate (PET), High temperature polymers, Bakelite, Melamine and other polymers. Molding process: Compression molding, transfer molding, injection molding, RIM, blow molding, rotational molding, thermoset molding, Extrusion, film extrusion, casting, coating, foaming, forming laminates.

UNIT II: Paint and Adhesives

A) Paints and Pigments: Introduction, preparation, and uses of white lead, zinc white, ultramaine, carbon black, lithophore, red lead, chrome green. Manufacture of paints, characteristics of a good paint, paint failure, varnishes, sprit varnishes, oleoresins, and varnish and paint industries in India.

B) Adhesives: Introduction, theories of adhesion, advantages and disadvantages of using adhesives, chemistry and uses of adhesives, natural product-based adhesives, pressure sensitive adhesives, hot melt adhesives, solvent and emulsion-based adhesives.

Unit III: Science of corrosion and corrosion control

Introduction, economic aspects of corrosion, theories of corrosion, factors affecting corrosion, Evans diagram, thermodynamics of corrosion, Fourbaix diagram, corrosion testing techniques, Evaluation of corrosion effect: XRD, ESCA, FTIR surface techniques. Corrosion Prevention methods: Corrosion inhibitors, protective coating, cathodic and anodic protection. Corrosion problem in India.

Unit IV: Sensor technology

Introduction, recent trends, classification of sensors, Elector analytical sensors, sensor electrodes, Metal membrane electrode sensors, Ionic Conductors, Wi-Fi technology, thin and thick film sensors, Nanosensors, Biosensors, Application of sensors in Industry.

Reference Books:

1. Zaki Ahmad, Principles of Corrosion Engineering and Corrosion Control; Butterworth-Heinemann, publisher 2006.

15 hrs.

15hrs.

15 Hrs.

15 Hrs.
- Ravve, Principles of Polymer Chemistry, 3rd edition, Springer New York, NY, 2012.S. Glastone: Physical chemistry
- Jacob Fraden, Handbook of Modern Sensors: Physics, Designs, and Applications 5th Edition, Kindle Edition, 2015
- <u>Ashish Bagwari, Geetam Singh Tomar, Jyotshana Bagwari, Jorge Luis Victória</u> <u>Barbosa, Musti K.S. Sastry</u>, Advanced Wireless Communication and Sensor Networks: Applications and Simulations, Chapman and Hall/CRC; 1st edition (12 July 2023)
- 5. Pietro Pedeferri, Corrosion Science and Engineering 2018.
- P. Ghosh, Polymer Science and Technology, Plastics, Rubbers, Blends and Composites, 3rd Edition, Tata McGraw Hill Education Private Ltd., New Delhi, 2011.
- Amiya Kumar Lahiri , Applied Metallurgy and Corrosion Control: A Handbook for the Petrochemical Industry (Indian Institute of Metals Series), Springer; 1st ed. 2017 edition (8 September 2017)
- 8. A.D. Wilson, J. W. Nicholson and H.J. Prosser, Surface Coatings-2 Springer; Softcover reprint of the original 1st ed. 1988 edition (26 September 2011)
- D. Patranabis: Sensor and Transducers, second edition, PHI Learning; 2nd edition (1 January 2003.
- 10. Industrial Chemistry by B.K. Sharma.

Course Outcomes:

Students will be able to

- CO1 How to prepare various commercial industrial polymers such as HDPE, LDPE, PET, SBR, and PVC
- CO2 Get knowledge regarding preparation of paints and adhesives.
- CO3 Brief description of corrosion science and prevention methods of corrosion
- CO4 Get information about introduction, classification and applications of sensor technology

RP-INDCH405: Research Project

See Annexture-I for details.

NOTE: Study tour is compulsory for M.Sc. Part- II Students in Sem-IV to visit Chemical Industries in India.

Major Electives (Choose any One)

M.Sc. II, SEM-III

Students of Inorganic/Organic/Physical/Analytical/Applied/Industrial Chemistry shall choose any one of the following elective papers.

E-ICH304: Organometallic and Bioinorganic Chemistry

Unit I: Organotransition Metal Chemistry

Alkyls and Aryls of Transition Metals: Types, routes of synthesis, stability and decomposition pathways of alkyls and aryls of transition metals. Organocopper in Organic synthesis, Compounds of Transition Metal –Carbon Multiple bonds: Alkylidenes, alkylidynes, low valent carbenes and carbynes–synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on ligands, role in organic synthesis.

Unit-II: Transition Metal Pi-complexes

Carbon multiple bonds. Nature of bonding, structural characteristics & synthesis, properties of transition metal Pi-Complexes with unsaturated organic molecules, alkenes alkynes, allyl, diene, dienyl, arene and trienyl complexes. Application of transition metal, organometallic intermediates in oraganic synthesis relating to nucleophilic and electrophilic attack onligands, role in organic synthesis.

Unit III: Metal Compounds in Medicine

Medicinal use of metal complexes as antibacterial, anticncer, use of cis-platin as antitumor drug, antibiotics & related compounds. Metal deficiency and disease, iron deficiency, zinc deficiency and copper deficiency, Metal used for dignosis and chemotherapy with particular reference to anti-cancer drugs. Chelate therapy, chemotherapy with compounds of some nonessential elements; platinum complexes in cancer therapy. Antiviral activity of metal complexes. Gold containing drugs used in the therapy of Rheumatic-Arthritis, Gold complexes as anticancer drug. Lithium in psycho pharmacological drugs. Antimicrobial agents.

15 hrs.

15 hrs.

Unit-IV: Oxygen Transport and Storage

Heme proteins and oxygen uptake, structure and functions of haemoglobin, myoglobin, hemocyanins & hemerythrin. Perutz mechanism for structural changes in porphyrin ring system, Oxygenation and deoxygenation. Oxygen adsorption isotherm and cooperativity, physiological significance of haemoglobin, role of globin chain in gaemoglobin, Cyanide poisoning and treatment.

Reference Books:

- 1. Yamamoto, Organo Transition Metal Chemistry, Wiley (1986).
- 2. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals (4th edn.), John Wiley (2005).
- 3. A. J. Pearson. Metallo-Organic Chemistry, John Wiley & Sons (1985).
- M. Bochmann. Organometallics-I Complexes with Transition Metal-Carbon σ-Bonds, Oxford Chemistry Primers (1994).
- 5. Principles of Biochemistry, A. L. Lehinger, Worth Publications.
- 6. Biochemistry, L. Stryer, W. H. Freeman
- 7. Biochemistry, J. David Rawn, Neil Patterson.
- 8. Biochemistry, Voet and Voet, John Wiley.
- 9. Outlines of Biochemistry, E. E. Conn and P. K. Stumpt, John Wiley.
- D. F. Shriver, P. W. Atkins and C. H. Langford, Inorganic Chemistry, Oxford Univ. Press, 1990.

Course Outcomes (COs):

CO1: After successful completion of the course the students should be able to explain the synthesis, structure, bonding, properties and reactivity of Alkyls and Aryls of Transition Metals.

CO2: After successful completion of the course the students should be able to explain the synthesis, structure, bonding, properties and reactivity of Compounds of Transition Metal-carbon with Multiple bonds.

CO3: Students should be able to describe the role of metals in medicines, deficiency disorders of metals and use of platinum, gold and lithium compounds in the treatment of cancer, arthritis and psycho drugs, respectively.

CO4: At the end of the course student should be able to explain the natural proteins that carry dioxygen in various animals, the role of myoglobin and hemoglobin in carrying dioxygen in mammals and other non-heme proteins for oxygen uptake.

E-OCH304: Drug and Heterocycles

Part- A: DRUGS

UNIT-I: Drug Design and Antibiotics

A. Drug Design

Procedures followed in drug design, **factors affecting development of new drugs**, concepts of prodrugs and soft drugs, **Isosterism, bioisosterism,** Theories of drug activity, Quantitative structure activity relationship, QSAR theory, Concepts of drug receptors.

B. Study of Antibiotics

(i) Classification of antibiotics, (ii) Preparation of semi synthetic penicillin, (iii) Penicillin G, (iv) Penicillin V, (v) Conversion of penicillin into cephalosporin.

UNIT-II: Study of the Following Drugs

- a) Antimalerials: Trimethoprim, Amodiaquine
- b) Analgesic & Antipyretics: Meperidine, Aminopyrine, Diflunisal
- c) Anti- inflammatory: Oxyphenylbutazone, Indomethacin
- d) Antitubercular & antileprotic: Dapsone, Pyrazinamide, Ethionamide
- e) Anaesthetics: Lidocaine, Thiopental
- f) Antihistamines: Cyproheptadine, Cetirizine
- g) Psychoactive: Ethiosuximide, Glutethimide
- h) Antiinfective: Grisefulvin, norfloxacin
- i) Cardiovascular: Warfarim, Clofibrate, Quinidine, Methyldopa, Atenolol
- j) Anti-neoplastic: Recent development in cancer chemotherapy. Hormones and natural products. Synthesis of (i) Mechloraethamine, (ii) Cyclophosphamide, (iii) Mephalan, (iv) Uracils, (v) Mustards.
- k) Anti-AIDS: General study

15 hrs.

(5)

15 hrs.

(10)

UNIT	C-III: Study of following heterocycles 15 hrs.			
A)	Small ring heterocycles:			
	(5)			
	3 and 4 membered heterocycles: Synthesis and reactions of (i) aziridines, (ii) oxiranes,			
	(iii) thiranes, and (iv) azetidines.			
B)	Six membered heterocycles with one heteroatom:			
	(5)			
	Synthesis and reactions of (i) pyrilium salts, (ii) pyrones, (iii) coumarins, (iv)			
chi	romones.			
C)	Six membered heterocycles with two and more heteroatoms: (5)			
	Synthesis and reactions of (i) diazines (ii) triazines			
UNIT	-IV: Study of following heterocycles 15 hrs.			
A)	Benzolused live membered heterocycles:			
-	Synthesis and reactions of (1) benzopyrroles, (11) benzofurans and (111) benzothiophene			
B)	Benzofused heterocycles with two heteroatoms:			
	Synthesis and reactions of			
	(i) benzimidazole, (ii) benzthiazole and (iii) benzoxazole			
Refer	ence Books.			
1	Medicinal Chemistry Burger			
2	Medicinal Chemistry A. Kar. (Wiley East)			
3	. Principals of medicinal chemistry.W. O. Fove:			
4	. Text book of organic medical and pharmaceutical chemistry. Wilson, Gisvold &			
	Dorque:			
5	. Pharmaceutical manufacturing encyclopedia.			
6	D. Sriram, P. Yogeeswari: Medicinal Chemistry			
7	. An introduction to chemistry of heterocyclic compounds. R. M. Acheson :(
	Interscience).			
8	. Heterocyclic chemistry. Joule &Smith: (Van Nostrand).			

Part-B: HETEROCYCLES

- 9. Heterocyclic chemistry. R. K. Bansal: (Wiley E).
- 10. Principals of modern heterocyclic chemistry.L. A. Paquitte:
- 11. The structure and reactions of heterocyclic compounds.M. H. Palamer:
- 12. Advances in Heterocyclic chemistry. A. R. Katritzky: (A.P.).
- 13. Organic chemistry (Vol. 1& 2) Finar.
- 14. Outline of Biochemistry. Cohn & Stumpt
- 15. Introduction to the chemistry of enzyme action. Williams:
- The Organic Chemistry of Drug design and Drug action. R. B. Silverman Academic press.
- 17. Strategies for Organic Drug synthesis and Design. D. Lednicer, J. Willey.
- Heterocyclic Chemistry. Vol-1-3, R. R. Gupta, M. Kumar and V. Gupta, Springer Veriag.
- 19. The Chemistry of Heterocycles. T. Eicher and S. Hauptmann, Thieme
- 20. Heterocyclic Chemistry. J. A. Joule, K. Mills and G. F. Smith, Chapman and Hall
- 21. Heterocyclic Chemistry. T. L. Gilchrist, Longman Scientific Technical
- 22. Contemporary Heterocyclic Chemistry. G. R. Nikome and W. W. Poudler, Willey
- 23. An Introduction to Heterocyclic Compounds, R. M. Acheson, J. Willey
- 24. Comprehensive Heterocyclic Chemistry. A. R. Katritzky and C. W. Rees

Course Outcomes (COs):

CO No.	On completion of the course, students will be able to:		
CO1	To know about the drug design, history, and development of		
quantitative structure-activity relationship (QSAR). Also, learn			
	concept of drug receptors and the relationship between structure and chemical reactivity. Learn about different types of antibiotics.		
CO2	Study the various types of drugs like antimalarials, Anti-inflammatory,		
	anesthetics, Antitubercular, Tranquilizers cardiovascular, and		
	Antineoplastic drugs.		
CO3	Understand synthesis and reactions of five, six-membered		
	heterocycles.		
CO4	Learn the synthesis and reactions of diazines and triazines. Synthesis		
	of the reactions of azepines, oxepines & thiepines.		

E-PCH304: Solid State Chemistry

UNIT-I: The Solid State

Introduction, laws of crystallography, lattice types, X-ray diffraction, Bragg's equation, Miller indices, Bragg's Method, Debye-Sherrer method of X-ray for structure analysis of crystals, indexing of reflections, identification of unit cells from systematic absence in diffraction pattern, structure of simple lattice and X-ray intensities, structure factor and its relation to intensity and electron density, phase problem, procedure for an X-ray structure determination, Rietveld analysis, Problems.

UNIT –II: Solid State Reactions

General principle, types of reactions: Additive, structure sensitive, decomposition and phase transition reactions, tarnish reactions, kinetics of solid-state reactions, Mechanochemical methods for preparations of semiconductors. Co-precipitations reactions, factors affecting the reactivity of solid-state reactions.

UNIT –III: Electronic Properties and Band Theory

Metals, insulators and semiconductors, free electron theory and its applications, electronic structure of solids, band theory, band structure of metals, insulator, and semiconductors, doping in semiconductors, p- n junction, superconductors, organic semiconductors, charge carrier injection and transport, Optical properties of organic semiconductors, applications and devices involving optical properties, luminescence photoluminescence, effect of impurity levels on photoluminescence, light emitting diodes, luminous efficiency, photo-conduction and photoelectric effects, laser, principle of laser action, solid state laser and their applications, Problems.

UNIT-IV: Preparation of Materials

Purification and crystal growth, kinetics of nucleation, critical radius, principle of nucleation, crystal growth during casting, zone refining, growth from solution, growth from melt and preparation of organic semiconductors for device applications.

Crystal defect and Non-Stoichiometry: Classification of defects subatomic, atomic and lattice defect in solids. Thermodynamics of vacancy in metals, Thermodynamics of Schottky

15 hrs.

15 hrs.

15 hrs.

defects in ionic solids, Thermodynamics of Frenkel defects in silver halides. Calculation of number of defects and average energy required for defect.

Reference Books:

- 1. A guide to laser in chemistry by Gerald R., Van Hecke, Keny K. Karokitis
- 2. Principles of Solid-State Chemistry, H. V. Keer, Wiley Eastern,
- 3. Solid State Chemistry, N. B. Hannay
- 4. Solid State Chemistry, D. K. Chakrabarty , New Age International
- 5. An Introduction to Crystallography: F. G. Philips
- 6. Crystal Structure Analysis: M. J. Buerger 49
- 7. The Structure and properties of materials: Vol. III Electronic properties by John Walss
- 8. Electronic processes in materials : L. U. Azroff and J. J. Brophy
- 9. Chemistry of imperfect crystal: F. A. Krogen
- 10. Elements of X-ray Diffraction by B. D. Cullity, Addison-Weily.
- 11. Solid State Chemistry by A.R.West (Plenum)
- 12. Electronics made simple by Jacobwitz.
- 13. Principles of Physical Metallurgy, by Abhijeet Mallick,

Course Outcomes (COs):

The Solid-State Chemistry Course Outcomes. On completing the module students will be able to:

CO1: Demonstrate an ability to describe, with confidence, the features of the most common crystalline structures.

CO2: Demonstrate the ability to identify different bonding contributions in the solid state.

CO3: Demonstrate the ability to relate the crystalline structure with the bonding to predict materials properties.

CO4: Demonstrate assured ability to describe different defect structures in the solid state and how they affect the materials' properties.

CO5: Demonstrate thorough analytical skills associated with the need to pay attention to detail and develop an ability to manipulate precise and intricate ideas, to construct desired materials for various applications in the industry.

CO6: Demonstrate the ability to work independently for the preparation of solid materials and characterization.

E-ACH 304: Environmental Chemical Analysis and Control

UNIT-I: Sampling in analysis

15 hrs.

Definition, theory and techniques of sampling, sampling of gas, liquids and solids, Criteria of Good sampling, Minimization of Variables, transmission and storage of samples, high pressure ashing techniques (HPAT), particulate matter, its separation in gas stream, Filtering and gravity separation. Analysis of particulate matter like asbestos, mica, dust and aerosols etc

UNIT-II: Electrochemical and spectral methods Environmental analysis 15 hrs.

Introduction to instrumental techniques, principle instrumentation and applications with respect to environmental analysis of Conductometry, Potentiometry, Ion selective electrodes, Cyclic voltammetry, Amperometry, Coulometry, Atomic absorption spectrometry, Atomic fluorescence spectrometry, Inductively coupled plasma spectrometry, Turbidimetry, Non Dispersive Infrared Analysis (NDIR).

UNIT-III: Air and Water Pollutant Analysis

Chemistry of Air pollutants, characterization. source, methods of analysis of air pollutants; CO, CO2, NOX, NH3, H2S, SO2 etc. Monitoring Instruments, Potable and Industrial water, major and minor components, dissolved oxygen (DO) Chemical oxygen demand(COD) Biochemical oxygen demand (BOD) and their measurements. Analysis of Pd, Cd, Hg, Cr, As and their physiological manifestations. Quality of industrial waste water analysis for organic and inorganic constituents. Chemistry of odour and its measurements.

UNIT-IV: Organic Pollutants and Their Analysis

Sources, disposal, treatment and analysis of phenolic residues, methods of recovery of phenols from liquid effluents, Organomercurials and its analysis, Analysis of organochlorine pesticides, volatile organic pollutants and their analysis

Reference books:

- 1. A.K. De: Standard Methods of Waste and Waste water analysis.
- 2. P. M. S. Monk Fundamentals of Electroanalytical chemistry-John Wiley & Sons
- a. (2001) 3. Instrumental methods of chemical analysis H. Kaur

15 hrs.

- 3. S.M. Khopkar, Environmental Chemistry; Environmental pollution analysis
- 4. M.S. Creos and Morr, Environmental Chemical Analysis, American publication
- a. (1988)
- 5. A.K. De, Environmental Chemistry, New Age International publishers. Moghe and
- a. Ramteke, Water and waste water analysis: (NEERI)
- 6. A.C. Stern, Air pollution: Engineering control Vol. IV(AP)
- 7. P.N. Cheremisinoff and R.A. Young, Air Pollution controland Design. Hand Book
- a. Vol. I & II (Dekker)
- 8. R.B. Pohasek, Toxic and Hazardous waste disposal, Vol. I & II (AAS)
- 9. M. Sitting, Resources Recovery and Recycling, Handbook of industrial Waste.
- 10. B.K. Sharma, Industrial Chemistry.
- 11. S.P. Mahajan, Pollution Control in Process Industries.
- 12. R.A. Horne, Chemistry of our Environment.

Course Outcomes (COs):

- CO1: Students will acquire knowledge about sampling, criteria of good sampling, handling, preservation and storage of the samples, pretreatment and post treatment of samples.
- CO2: Students will acquire knowledge of conditions and strategies required during sampling and electrochemical and spectral methods for analysis of environmental samples.
- CO3: Students will learn about the air and water pollution, sources of pollution, typical parameters and properties (physical, chemical and biological) to be measured in air and water pollution with relevance to specific case studies.
- CO4: Students will be acquainted with organic pollutants and their analysis with special reference to pesticide analysis.

Major Electives (Choose any One)

M.Sc. II, SEM-IV

Students of Inorganic/Organic/Physical/Analytical/Applied/Industrial Chemistry shall choose any one of the following elective papers.

E-ICH 404: Energy and Environmental Chemistry

Unit I: Energy Conversion Devices

15 hrs.

15 hrs.

Fuel Cells: Working of Fuel Cells, Types of fuel cells, Current capabilities/uses, Fuel cell stacks and systems, Hydrogen as a fuel, Production of hydrogen: Electrolysis, Thermochemical Processes, Steam Reformer Processes, Water Gas Processes, Bosch Process, Biosynthesis and Photochemical Processes, Coal Gasification, Steam Iron Process, Partial Oxidation Processes. Storage, Transport, and Handling of Hydrogen.

UNIT II: Energy Storage Devices: Batteries

Li-ion batteries: Principle of operation, Battery components and design, Electrode materials (LiCoO₂, LiNiO₂, LiNi_{1/3}Mn_{1/3}Co_{1/3}O₂, LiMn₂O₄, LiFePO₄, graphitic carbon) their synthesis and characterization, Theoretical capacity, Energy density, power density, cycle life, Electrode and battery fabrication, Battery modules and packs, Li-polymer batteries and applications, Electrolytes for Li-ion batteries, All solid-state batteries. Future developments and beyond lithium batteries: Li-S battery, Li-Air battery, Advanced lead-acid batteries, Sodium-battery, Magnesium battery, Aluminium battery, Silicon battery, Battery Recycling Technologies.

UNIT III:

A) Waste Treatment

Electronic waste recycling programs, E-waste – non-recycling impacts, Materials Used in Manufacturing Electrical and Electronic Products, Solid Waste Management: Gas to Energy projects, Incandescent vs. compact florescent light bulbs, Value-added Material Recovery, Cost effective treatment of refractory organics,

B) Air and Water Pollution control

Control of NOx, SOx and particulate pollution, Sewage and industrial waste water treatment, water softening, municipal water purification.

8 hrs.

UNIT-IV:

A) Monitoring, sampling and Analysis of Air and water pollutants 8 hrs. Methods of monitoring and sampling of gaseous, liquid and solid pollutants, analysis of CO, CO_2 , NO_2 , SO_2 , H_2S , analysis of toxic heavy metals, Cd, Cr, Hg, As, Pb, analysis of anions SO_4^{2-} , PO_4^{3-} , NO_3^{-} , estimation of COD and BOD

B) Techniques in Environmental Analysis

7 hrs.

ND-IR Spectroscopy, FTIR, AAS, ICP-AES, GC, GC-MS, HPLC, Anodic stripping voltammetry with case studies

Reference Books:

- 1. Lithium ion Batteries: Basics and Applications, R. Korthauer, Springer
- Lithium ion Batteries: Fundamentals and applications, Yuping Wu, CRC Press, Taylor &

Francis group

- Lithium ion batteries: Materials, Technology and new applications, K. Ozawa, Wiley 30 Years of Lithium-Ion Batteries, Advanced Materials, M. Li et al., Vol 30, issue 33, 2018,1800561
- 4. Fuel Cell Fundamentals, R. O'Hayre, et al., John Wiley & Sons, 2016
- George Techobanoglous et al, "Integrated Solid Waste Management" McGraw Hill, 1993.
- 6. Environmental Chemistry, H. Kaur, PragatiPrakashan, 10th edition 2016.
- 7. Environmental Pollution, A. K. De
- 8. Environmental Pollution Analysis, S. M. Khopkar
- Compendium of R&D Projects, Waste Management Technologies (WMT) Programme, Technology Development and Transfer Division, Department of Science and Technology, New-Delhi 2018-2019.
- 10. Environmental Waste Management, Ed. Ram Chandra, CRC Press 2015, 1st Edition
- Electronic Waste Management, RSC Publishers, Editors: R E Hester, R M Harrison, 2009

Course Outcome (COs):

CO1: At the end, students will be able to: Learn basic concepts of solid waste management, beginning from source generation to waste disposal.

CO2: Students should be able to-Characterize the solid waste in terms of hazardous waste components; impact of waste management on health and environment; understand steps towards solid waste management-waste reduction at source, materials and resource recovery/recycling, treatment and disposal techniques.

CO3: After completion of the course student will be able to explain the advanced energy conversion devices such as Fuel cells, and the various techniques involves in the production of Hydrogen (future fuel).

CO4: Students will be able to demonstrate the reactions involved in the advanced energy storage devices, can predict the theoretical energy storage capacities of such devices, and understand the chemistry of various batteries.

E-OCH404: Applied Organic Chemistry

UNIT-I: Study of Agrochemicals and Perfumes

A) Agrochemicals

(i) Organochlorine pesticides: Introduction, synthesis, and mode of action of endrin, aldrin, dieldrin. (ii) Herbicides: Synthesis and mode of action of Triazines, triazoles, pyridazinones, and bipyridylium compounds: diquat, paraquat. (iii) Juvenile hormone: introduction & structures JHA importance synthesis, IPM

B) Synthesis and applications of perfumery

2-Phenylethanol, vanillin, and other food flavors, synthetic musk, and ionones.

UNIT-II: Unit processes

Introduction to unit operation and unit processes. Nitration: Introduction, Nitrating agents, kinetics and mechanism, oxynitration, typical industrial nitration process.

Amination: Introduction, Bechamp reduction. Halogenation: Introduction, Kinetics and mechanism, catalytic chlorination, manufacturing process for chlorobenzene and monochloroacetic acid. Sulfonation- Introduction, sulphonating agents, kinetics and mechanism, manufacturing process for benzene sulphonic acid.

UNIT-III: Dyes and Intermediates

Classification and synthesis of important dye intermediates by using nitration, sulphonation, diazotization reactions. Synthesis of Nitro dyes, xanthenes, reactive dyes, fluorescent brightening

15 hrs.

15 hrs.

(8)

15 hrs.

(7)

agents, thermal sensitive dyes, dispersed dyes and reactive dyes.

UNIT-IV: Polymers

Mechanism of polymerization. Industrial process for synthesis of polyethylene, acrylonitrile, acrylate and methacrylate polymer, biomedical polymer, polymer processing, Plasticizers and anti-oxidants for polymers,

Reference Books:

- 1. Allan: Colour Chemistry
- 2. K. Venkataraman: Chemistry of Synthetic Dyes Vol-1 to 7
- 3. G. R. Chatwal: Synthetic dyes
- 4. Abrahart: Dyes & their intermediates
- 5. N. N. Melikov: The Chemistry of Pesticides and formulations
- 6. K. H. Buchel: Chemistry of Pesticides.
- 7. R. Clemlyn: Pesticides
- 8. K. H. Buchel: Chemistry of Pesticides
- 9. H. R. Alcock and F. W. Lambe: Contemporary Polymer Chemistry
- 10. J. M. G. Cowie, Blackie: Physics & Chemistry of Polymers
- 11. I. M. Campbell: Introduction to Synthetic Polymers
- 12. A. L. Gupta: Polymer Chemistry
- 13. M. S. Bhatnagar: A textbook of Polymers
- 14. F. W. Billmeyer: Textbook of Polymer Science

Course Outcomes (COs):

CO On completion of the course, students will be able to:

- No.
- CO1 Learn about the synthesis and uses of different types of Agrochemicals such as Carbamates, organophosphorous insecticides, and Natural and Synthetic Pyrethroids. They will learn the synthesis of some plant growth regulators as well as applications of Juvenile hormones and Pheromones.
- CO2 Learn about the perfumery compounds, commercial process, preparation and importance of essential oils. Also learn the synthesis of 2 phenyl ethanol, yara-yara, vanillin, synthetic musk, jasmine, ionone etc. from citral, phenyl acetate ester, benzyl acetate ester.

- CO3 Understand the classification, and synthesis of azo dyes, reactive dyes, optical brighteners, dispersed dyes.
- Understand the mechanism of polymerization. Also, study about the CO4 manufacturing processes of synthetic rubber plasticizers, and anti-oxidents required for natural polymers like starch and cellulose. They will get the knowledge about the Oxo and Wacker process necessary for Soap and Synthetic detergents.

E-PCH404: Surface Chemistry

UNIT-I: Surface Chemistry of Interfaces

Types of interfaces, liquid-vapour interface, surface tension and interfacial tension, surface tension across curved surfaces, capillary action, methods of determination of surface tension, vapor pressure of droplet (Kelvin equation), surface activity and adsorption phenomenon, Trube's rule, liquid-liquid interfaces, work of cohesion and adhesion, surface spreading, spreading of one liquid on the surface of other liquid, spreading coefficient and derivation for its relation with surface tension, surface films on liquids, criteria for spreading of one liquid on another. Experimental techniques for the study of monomolecular films, states of monomolecular films reaction on monomolecular films, heterogenous catalysis.

UNIT -II: Solid-Liquid and Solid - Solid interfaces

Solid-liquid interfaces, Introduction, wetting phenomenon, contact angle and wetting, heat of wetting, methods of determination of contact angle, contact angle hysteresis, wetting agents, selective wetting, applications in detergency, and pesticide affectivity, solid-solid interfaces, introduction, surface energy of solids, adhesion, and adsorption, sintering and sintering mechanism, Tammann temperature, importance of impurities, surface structure and surface composition. Friction and lubrication, mechanism of lubrication, solid state lubricants.

Unit-III: Solid-gas interfaces

Adsorption, mechanism of adsorption, adsorption of gases by solids, surface area measurement, factors affecting on adsorption, experimental methods of determining gases adsorption, adsorption of solutes from solution, heat of adsorption, measurement of heat of adsorption,

15 hrs.

15 hrs.

Chemisorption: kinetics of chemisorption, heat of chemisorption, surface film, Catalysis of gases reaction by solid surface, One reactant gases slightly/ strongly/ moderately adsorbed, Retarded reaction, ion exchange adsorption, Applications.

UNIT- IV: Colloids and emulsion

Colloidal solution, classification of colloids, Theories of origin of charge on sol particles, determination of charge on a colloidal particle, stability of sols, properties of colloids, spontaneous ageing of colloids, factors affecting on the spontaneous ageing, theories of spontaneous ageing, coagulation, kinetics of coagulation.

Emulsion: Types of emulsion, preparation, properties, characteristics, identification test between two types of emulsions, emulsifiers, demulsification.

Gels: classification, methods for the preparation of gels, properties of gels, applications of colloids.

Reference Books:

- 1. Physical chemistry of surfaces: A. W. Adamson.
- 2. Introduction to colloid and surface chemistry by D. J. Shaw. 58
- 3. Surface chemistry by J. J. Bikermann

4.The Surface Chemistry of Solids, by S.J.Gregg, Second Edition, Chapman & Hall Ltd. London.

5. Advanced Physical Chemistry, by Gurdeep Raj, Goel Publishing House, Krishna Prakashn Media (P) Ltd., Meerut-250001(UP)

6. Physical Chemistry by Pahari S. New Central Book Agency (P) Ltd. Kolkata.

7. Advanced Physical Chemistry J.N. Gurtu, A. Gurtu. 11th Edition Pragati Prakashan.

8. Advanced Physical Chemistry D N Bajpai S Chand Publications

 8. Essentials of Physical Chemistry by Arun Bahl, B S Bahl, G D Tuli . S Chand Publications 9. Principles of Physical Chemistry by S H Maron and C F Prutton
10. Physical Chemistry, P. W Atkin.

Course Outcomes (COs):

After completion of course student will able to understand

CO1: Understand concepts of solid-liquid, solid-gas, liquid-gas interfaces.

CO2: Apply fundamental principles of chemistry to chemical processes occurring at interfaces.

CO3: Apply spectroscopic methods to study interfaces and interfacial phenomena.

CO4: Learning and understanding the importance, applications, and basic aspects of surface chemistry.

CO5: The course focuses on the fundamentals of surface chemistry, with the main emphasis on solid surfaces in contact with gas phase.

CO6: Adsorption, desorption and colloidal applications of surface chemistry are able to apply this knowledge in understanding and designing surface chemistry processes.

E-ACH404: Applied Analytical Chemistry

UNIT-I: Spectrochemical Methods of Analysis

Introduction to spectrochemical methods. Electronic spectra and molecular structure, NIR spectrometry for non-destructive testing. Solvents for spectrometry, FTIR spectrometer, fluorometry, optical sensors. Analysis of ores -bauxites, dolomites, monazites. Analysis of Portland cement.

UNIT-II: Analysis of metals and alloys

Foundry materials, ferroalloys, and special steels, slags, fluxes. Analysis of alloys, bronze, brass, Alnico and Nichrom.

UNIT-III: Analysis of soil and fertilizers

Method of soil analysis, soil fertility and its determination, determination of inorganic constituents of plant materials, Chemical analysis as measure of soil fertility, analysis of fertilizers, applications.

UNIT-IV: Analysis of Commercial materials

Analysis of explosive materials, TNT, RDX, lead azide, EDNA (ethylene dinitramine). Analysis of conducting polymer, resins and rubber. Analysis of luminescent paints, Analysis of lubricants and adhesive.

Reference Books:

1. Hillebrand Lhundel, Bright and Hoffiman, Applied Inorganic Analysis, John Wiley.

15 hrs.

15 hrs.

15 hrs.

- 2. Snell and Biffen, Commercial Methods of Analysis.
- 3. P. G. Jeffery, Chemical Methods of Rock Analysis, Pergamon.
- 4. Buchel, Chemistry of Pesticides. J Wiley.
- 5. Rieche, Outlines of Industrial Organic Chemistry, Butter Worth.
- 6. F. A. Henglein, Chemical Technology, Pergamon.
- 7. Kent, Riegl's Industrial Chemistry, Rainhold.
- 8. Chopra and Kanwar, Analytical Agriculture Chemistry, Kalyani Publishers.
- 9. Aubert and Pintes, Trace Elements in Soils.
- 10. Bear, Chemistry of Soil.
- 11. Hauson, Plant Growth Regulators, Noyes.
- 12. P. G. Jeffery and D.J. Hatchinson, Chemical Methods of Rock Analysis.

13. F. J. Weleher, Standard Methods of Chemical Analysis, A Series of Volumes Robert and Krigeger Publishing Company.

14. I. M. Kolthoff and PJ Ewing, Treatise o Analytical Chemistry, A series of Volumes.

15. R. D. Reeves and R.R. Brooks, Trace element Analysis of Geological Materials, John Wiley & Sons New Dehli.

16. W. M. Johnson and J.A. Maxwell, Rock and Mineral Analysis, John Wiley and Sons, New York.

W. F. Hildebrand, GHC Landell and HA Brighot, Applied Inorganic Analysis, John Wiley 2nd Ed.

18. K. J. Das, Pesticide Analysis (MD).

Course Outcomes (COs):

- CO1: The students will acquire knowledge of analysis of metals, alloys, minerals and ores commonly used in the industry.
- CO2: The students will be acquainted with the analysis of real samples like cement, plaster of Paris, different commercial ores, soil composition, soil fertility, fertilizers etc using conventional and instrumental methods of analysis.
- CO3: Students will also gain the knowledge of analysis of commercial materials, explosives, polymers, resins, rubber, luminescent paints, lubricants and adhesives.
- CO4: These would offer opportunity to the students to get employment in industries for quality assurance and quality control (QA-QC) of the product.

Annexture-I

Research Project Paper Guidelines for all specializations

(Inorganic, Organic, Physical, Analytical, Applied and Industrial Chemistry)

<u>Semester III</u>

RP-ICH306, RP-OCH306, RP-PCH306, RP-ACH306, RP-APCH306, RP-INDCH306 Credits= 04, 120 Hours, 100 Marks

- The students should write synopsis of proposed research work.
- The students should perform detail literature survey related to research problem.
- The students should write review article related to research problem.
- It is expected to publish the review article either in Shivaji University Journal or peer reviewed journals.
- The students should design the problem and start experimental work. The students should complete at least 25% of their experimental work during the semester III and the same work to be continued in semester IV.
- The student should submit the spiral bound copy of research work carried out during semester III including the synopsis, research proposal, review article and certified progress report.
- The Research Project will be examined jointly by internal and external examiners during the practical examination at the end of the semester.
- The students should present their work during the evaluation in the form of power point presentation (PPT).

Sr. No.	Description	Marks
1	Synopsis	10
2	Research Proposal	20
3	Review article on proposed work	20
4	Daily Lab notebook record	10
5	Progress of Experimental work	20
6	Quality and effectiveness of presentation	20
	Total	100

• Marking Scheme:

Broad guidelines for preparation of synopsis

A. The proposed synopsis for research should be self contained and should cover the rationale for carrying out research.

- B. There should not be repetition of the work or topic or theme.
- C. The synopsis of the proposed research shall contain the following points :
- 1. Title of the Research Proposal
- 2. Motivation with reasoning and significance of the proposed research
- 3. Statement of the problem
- 4. Review of the relevant literature
- 5. Objectives of the study
- 6. The methodology comprising
- a. Methods of research
- b. Sampling design and assumptions
- c. Conceptual framework if any

d. Research design (explanation of how research is being conducted and the tools used for the same)

e. Methods of data collection

f. Methods of data analysis (use of parametric and non-parametric tools and techniques as the case may be)

- 7. Expected outcome
- 8. Bibliography.

Template for Research Proposal

- Title
- Introduction
- Origin of the research problem
- Interdisciplinary relevance
- Review of Research and Development in the Subject
- Significance of the study
- Objectives
- Plan of research work

M. Sc. II Semester IV

RP-ICH405, RP-OCH405, RP-PCH405, RP-ACH405, RP-APCH405, RP-INDCH405 Credits= 06, 180 Hours, 150 Marks

- The student should submit the final bound dissertation/thesis copy of research work carried out during semester III and IV.
- It should include title page, certificate, declaration, acknowledgement, abbreviations, index, abstract, introduction, experimental section, results and discussion, conclusions, references, participation in conferences/seminars and publications if any.
- The students should present their work during the evaluation in the form of power point presentation (PPT).

Sr. No.	Description	Marks
1	Dissertation/thesis bound copy	30
2	Quality of work (Innovative concepts, social relevance, extent of work etc.)	50
3	Publications	20
4	Participation in conferences	10 maximum
	a) Oral/Poster Presentation (10 marks)	
	b) Only attended (7 marks)	
5	Final Dissertation/thesis defence	40
	Total	150

• Marking Scheme:

Note: The Project will be examined jointly by internal (Project Supervisor) and external examiners (preferably Associate professor and above with Ph. D.) at the end of the semester. The project can be given individually or a maximum group of three students is allowed. (Not more than three students allowed).

M.Sc. II Syllabus (NEP-2020)

To be implemented from June 2024 onwards Semester III & IV

Nature of Question paper

Total Marks 80

Instructions: 1) Attempt in all five questions.

- 2) Question No. 1 is compulsory.
- 3) Attempt any two questions from Section-I and any two questions from Section-II.
- 4) All questions carry equal marks. Figures to right indicate marks.

Q.1 Solve the Following (Compulsory1 Mark each) Marks 16

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Section I

Q.2. Two sub questions (8 marks each) or Three sub question (6+6+4 marks) = 16 Marks

Q.3. Two sub questions (8 marks each) or Three sub question (6+6+4 marks) = 16 Marks

Q. 4 Two sub questions (8 marks each) or Three sub question (6+6+4 marks) = 16 Marks

Section II

Q.5. Two sub questions (8 marks each) or Three sub question (6+6+4 marks) = 16 Marks

Q.6. Two sub questions (8 marks each) or Three sub question (6+6+4 marks) = 16 Marks

Q.7. Writes notes on **any four** of the following (Out of Six)16Marksa)

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M.Sc. II Syllabus (NEP-2.0) To be implemented from June 2024 onwards Nature of Practical Examination

Semester III

Practical Paper V = 50 marks

Q. 1 Major Experiment =25 marks

Q. 2 Minor Experiment =15 marks

Q. 3 Oral= 5 marks

Q.4 Journal =5 marks

Number of Examination Days = 01