DR. BABASAHEB AMBEDKAR MARATHWADA UNIVERSITY

CIRCULAR NO.SU/M.Sc./Phy.Chem./32/2022

It is hereby inform to all concerned that, the syllabi prepared by the Committee and recommended by the Dean, Faculty of Science & Technology, the Hon'ble Vice-Chancellor has accepted **the syllabus of M.Sc. Physical Chemistry IIIrd & IV th semester under the scheme of Choice Based Credit & Grading System** in his emergency powers under section 12(7) of the Maharashtra Public Universities Act, 2016 on behalf of the Academic Council as appended herewith.

This is effective from the Academic Year 2022-23 and onwards.

All concerned are requested to note the contents of this circular and bring the notice to the students, teachers and staff for their information and necessary action.

University Campus,
Aurangabad-431 004.
REF.NO.SU/2022/14100-108
Date:- 21.10.2022.

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Deputy Registrar,
Academic Section

Copy forwarded with compliments to :-

1] **The Principal of all concerned Colleges,**
Dr. Babasaheb Ambedkar Marathwada University,
2] **The Director, University Network & Information Centre, UNIC, with a request to upload this Circular on University Website.**

Copy to :-

1] The Director, Board of Examinations & Evaluation, Dr.BAMU,A'bad.
2] The Section Officer,[M.Sc.Unit] Examination Branch,Dr.BAMU,A'bad.
3] The Programmer [Computer Unit-1] Examinations, Dr.BAMU,A'bad.
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5] The In-charge,[E-Suvidha Kendra], Rajarshi Shahu Maharaj Pariksha Bhavan, Dr.BAMU,A'bad.
6] The Public Relation Officer, Dr.BAMU,A'bad.
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DR. BABASAHEB AMBEDKAR MARATHWADA UNIVERSITY,

AURANGABAD.

DEPARTMENT OF CHEMISTRY

NAAC Re-accredited 'A' Grade

Curriculum

M. Sc. Physical Chemistry

(Semester III & IV)

Choice Based Credit and Grading System

(Common for University Department and All Colleges)

Effective from: June 2022

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University, Aurangabad

The following will be the Choice Based Credit and Grading System structure of revised syllabus for M. Sc. III & IV semester Physical Chemistry effective from June 2022-23.

Semester	Paper Nos.	Title of Paper	Credits	Teaching (hr)/week	Marks		Total Marks
					Internal	University Examination	
III-Semester	CHESC-313	Structural elucidation by spectral methods	04	04	20	80	100
	CHEP- 314	Solid state chemistry	04	04	20	80	100
	CHEP-315	Thermodynamics	04	04	20	80	100
	CHEP -316	Advanced electrochemistry	04	04	20	80	100
IV semester	CHEP-417	Surface and magnetochemistry	02	02	20	80	50
	CHEP -418	Polymer chemistry	04	04	20	80	100
	CHEP -419	Chemical dynamics and catalysis	04	04	20	80	100
	CHEP - 420(A)	Nano chemistry **,OR**	04	04	20	80	100
	CHEP - 420(B)	Instrumental methods of chemical analysis, **OR**	04	04	20	80	100
	CHEP - 420(C)	Advanced Quantum chemistry	04	04	20	80	100
III & IV Semester Laboratory Course	CHEP-421	Laboratory course	4.5	4.5	N.A.	50	50
	CHEP-422	Laboratory course	4.5	4.5	N.A.	50	50
	CHEP - 423	Research project (Experimental)	4.5	4.5	N.A.	50	50
	CHEP - 424	Research project (Dissertation Presentation and Seminars)	4.5	4.5	N.A.	50	50

Practical examination of III and IV Semester will be conducted at the end of fourth semester theory examination.

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CHESC-313: Structural elucidation by spectral methods

04 Hrs/Week **Credits: 04** **Marks 100**

UNIT-I: Nuclear Magnetic Resonance Spectroscopy (^{1}H NMR) **[12hrs]**

Elementary ideas (Recapitulation); Spin-spin couplings, Different types of couplings, factors affecting on coupling constants, Karplus equation, Spin systems (AB, AX, ABX, AMX), Rate processes, spin decoupling, shift reagents, Nuclear Overhauser effect (NOE), INEPT and INADEQUATE.

UNIT-II: ^{13}CNuclear Magnetic Resonance Spectroscopy **[12hrs]**

Elementary ideas, instrumental problems, chemical shifts (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbons); Effect of substituents on chemical shifts.

UNIT-III: Mass Spectroscopy **[12hrs]**

Introduction, ion production (EI, CI, FD and FAB), ion analysis, ion abundance, factors affecting on fragmentation, fragmentation of different functional groups, molecular ion peak, isotopic peaks, metastable peak, Nitrogen rule, McLafferty rearrangement, Retro-Diels-Alder reaction.

UNIT-IV **[12hrs]**

Problems based on joint applications of UV, IR, ^{1}H NMR, ^{13}C NMR and Mass spectroscopy.

UNIT-V **[12hrs]**

Mossbauer spectroscopy: Principle, factors affecting the line position and shape, isomer effect and Quadrupole splitting iron salt like compounds, complexes, carbonyl compounds (temperature dependence of isomer shift and Quadrupole splitting in simple compound and coordination, polynuclear complexes), Numericals. **Electron Spin Resonance Spectroscopy:** Introduction, principle of ESR spectroscopy, presentation of spectrum, hyperfine splitting in various structures, hyperfine splitting diagram of representative examples, factors affecting the magnitude of 'g' values, Zero field splitting, Kramer's degeneracy, Anisotropy in the hyperfine coupling constant, electron delocalization, instrumentation and applications.

Reference Books:

1. Introduction to Spectroscopy: D. L. Pavia, G. M. Lampman, G. S. Kriz
2. Spectrometric Identification of Organic Compounds: R. M. Silverstein & F. X. Webster
3. ^{13}C NMR Spectroscopy: G. C. Levy, R. L. Lichter, G. L. Nelson
4. Spectroscopic Methods in Organic Chemistry: D. H. Williams & I. Flemming
5. Absorption Spectroscopy of Organic Compounds: V. M. Parikh

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6. Mass Spectrometry: K. G. Das & James
7. Coordination Chemistry by Experimental Methods: K. Barger
8. Coordination Chemistry vol. I: E. Martell
9. Physical Methods for Chemistry: R. S. Drago
10. Structural Methods in Inorganic Chemistry: E. A. V. Ebsworth& D. W. H. Rankin
11. Organic Structure Analysis: Philips Crews

CHEP - 314 : Solid state chemistry

04 Hrs/Week **Credits: 04** **Marks 100**

Unit-I: Solid State Reactions **12 Hrs**

General Principles, Classification, Wagner reaction mechanism, Laws governing nucleation, Growth of nuclei, improving reactivity of solids, co precipitation as a precursor to solid state reactions, Kinetics of solid state reactions, factors affecting the reactivity of solid state reactions. General principles of growing single crystals, General conditions for crystal growth, solvent properties and saturated solutions, methods for growing crystals, slow evaporation, slow cooling, variation on slow evaporation and slow cooling, solvent diffusion, reactant diffusion, sublimation and seed crystals.

Unit-II: Imperfections in solids **12 Hrs**

Perfect and imperfect crystal, Point defects, Stiochiometric defects, Schottky and Frenkel defects. Thermodynamics of their formation, colour centers. Nonstoichiometric defects. Metal excess and metal deficiency defects. Line imperfections, edge dislocation and screw dislocation, Burger's circuits. Surface imperfection, `grain boundries and stacking faults.

Unit-III: Semiconductors and their devices **12 Hrs**

Intrinsic and extrinsic semiconductors, semiconductors materials and their fabrication, semiconductors devices p-n junctions, properties of p-n junctions, semiconductors diode as rectifier, Filters circuits, Zener diode as a voltage stabilizer, transistors transistor as an amplifier Super conductivity: conventional super conductors, organic super conductors (organic metals), fullerence, high temperature super conductors, organic charge transfer complexes Applications.

Unit-IV: Theories of solid state and properties of solids **12 Hrs**

Free electron theory, Conduction by free electrons, Band theory, refinement to simple band theory, band structure of metals. Insulator and semiconductors. Generation of x-rays, interaction of x-rays with matter, scattering and diffraction, Bragg's law, Miller indices, General instrumentation, Bragg's method, single crystal method, Debye-Scherrer method, Identification of unit cells from systematic absences, x-ray intensities and structure determination, structure factor and its relation to electron density and intensity, indexing of lattice planes in a cubic

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system, structure of NaCl and KCl, Avogadro's number from cubic lattice dimensions, applications of x-ray diffraction.

Unit-V: Ceramics **12 Hrs**

Introduction, major component of ceramics, clays, silica, feldspar, clay minerals, classification of clay minerals, properties of clay minerals, pillared clays, principal of pillaring, variety of pillaring species, modification of pillared clays, preparation of pillared clays, catalytic applications.

Reference Books

1. Solid State chemistry and its Applications-A. R. West (John Wiley and sons)
2. Principles of Solid State –H.V. Keer (Wiley Eastern Limited)
3. Material science and Engineering-V.Raghavan (prentice Hall of India)
4. Principles of Electronics- V.K.Metha (S.Chand and co.)
5. Engineering chemistry –P.C. Jain and M. Jain (Shanpat Rai and Sons)
6. Industrial chemistry –B.K. Sharma (Goel publishing House)
7. Selected topics in solid state physics vol.12 The growth of crystals from liquids
8. J.C. Brice, North Hollond/American Elesvier(1973)
9. Chemistry of imperfect crystal-F.A. Krogen
10. Crystals and Crystal Growing, Alan Holden and Phylis Singer, Anchor Books Doubleday, New York, 1960
11. X-ray Structure Determination A Practical Guide, 2nd edition George H. Stout and Lyle H. Jensen, John Wiliey & Sons, New York. 1989.

CHEP - 315 : Thermodynamics

04 Hrs/Week **Credits: 04** **Marks 100**

Statistical Thermodynamics

Unit-I: Introduction **12hrs**

Ensembles-canonical, grand canonical and micro canonical Combinatorial problems, Thermodynamics probability and most probable distribution, Stirlings approximation, distribution laws, the law of equipartition of energies. Quantum statistics- Max Well-Boltzmann, Bose-Einstein and Fermi-Dirac, limit and applicability of various distribution laws.

Unit-II: Molecular Partition function **12hrs**

Partition function, Expression for translational, rotational, vibrational and electronic partition functions, Third law of thermodynamics and partition function, Numerical problems.

Unit-III: Application to chemical systems **12hrs**

Partition function and Thermodynamic functions, Sackur-Tetrode equation (derivation), determination of equation of state of an ideal gas. Internal rotation, residual entropies, heat capacity of solids: Einstein model, Debye modification (model), characteristic temperature, statistical mechanics of solutions ideal and nonideal.

Unit-IV: Applications to quantum systems **12hrs**

Nuclear spin statistics, ortho and para nuclear states, ortho and para hydrogen.Fermi energy, Fermi energy of electron gas in metals, Plancks distribution law and radiation, Bose-Einstein degenerate gas (He gas).

Unit-V: Irreversible Thermodynamics **12hrs**

Postulates, entropy production in heat, entropy production in matter flow, entropy production in chemical reactions, Onsager's theory, microscopic reversibility and Onsager's reciprocity, stationary states and entropy production, Prigogine's principle of minimum entropy, application to thermoelectric effects-Seeback and Peltier effect.

Reference Books

1) Statistical Thermodynamics, Donaid A. Mc Qurrie, Harper & Row, New York 1973.
2) Statistical Thermodynamics, M.C. Gupta, Wiley Eastern Ltd. New Delhi.
3) Elements of Statistical Thermodynamics, L. K. Nash Addison Wesley, Menlo Park, 1972.
4) Physical chemistry, P. W. Atkins, ELBS
5) Non Equilibrium Thermodynamics, Progogine Kalyani Publication.
6) Thermodynamics and Non Equilibrium Thermodynamics, Gurudeep & Raj.

CHEP -316 : Advanced electrochemistry

04 Hrs/Week **Credits: 04** **Marks 100**

Unit -I: Oxidation - Reduction Systems: **12 Hrs**

Oxidation potentials, reversible ox-red systems, determination of standard ox-red potentials, variation of ox-red potential, ox-red equilibria, ox-red systems in analytical chemistry, ox-red indicators, two stage ox-red , semiqinone formation constant. Numericals.

Unit-II: Bio- electrochemistry and Electrocatalysis **12 Hrs**

Donnan membrane equilibrium, membrane potential, theories of membrane potential,introduction to electrocatalysis, relative power of electrocatalysts, mechanism of electrocatalysis, bioelectro catalysis, immobilization. application of enzymes on electrodes.

Unit-III: Electrodeposition **12 Hrs**

Introduction, the electrogrowth of metals on electrodes , the reaction pathway for electro deposition, surface diffusion of ions, cathodic deposition of metals from solutions, factors affecting cathodic deposition of metals, electrochemical dissolution and passivity of metals, anodic dissolution of metals, film and adsorption theories of passivity.

Electroplating of metals, mechanism, throwing power of an electroplating bath, factors affecting throwing power, typical electrodeposition processes, and applications of electroplating of metals. Numericals.

Unit-IV: Polarization and Overpotentials **12 Hrs**

Polarization, concentration polarization, decomposition potentials, over voltage, hydrogen, oxygen and metal overvoltages, types of overvoltages, factors affecting overvoltages, experimental determination of decomposition potential and overvoltage, Tafels theory and Tafel equation, simultaneous deposition of metals .Numericals

Unit-V: Conversion and storage of electrochemical energy **12 Hrs**

Introduction of storage cells, fuel cells, solar cells Types of storage cells (batteries), measure of cell performance, charging and discharging, introduction of classical batteries, modern batteries –zinc-air , nickel-metal oxide and lithium batteries.

Brief history of fuel cells, efficiency of fuel cells, hydrogen-oxygen fuel cell, phosphoric acid fuel cell, direct methanol and biochemical fuel cells; Solar cells introduction, principle and working of solar cells, advantages.

Reference Books:

1) Modern Electrochemistry, Vol 1,2A and 2B, John O" M Bokris
2) An Introduction to Electrochemistry, Samuel Glasstone.
3) Theoretical Electrochemistry, L.Antropov.
4) Advanced Physical Chemistry, Gurtu and Gurtu.
5) Principles of Physical Chemistry, Puri,Sharma and Pathania.
6) Text Book of Physical Chemistry, S. Glasstone
7) Physical Chemistry, Robert J. Silbey.
8) Physical Chemistry, G.K.Vemulapalli.
9) Physical Chemistry, Maron and Pruton.

A S Rajbhoj

10) Physical Chemistry, P.W. Atkins

CHEP- 417: Surface and magnetochemistry

04 Hrs/Week **Credits: 04** **Marks 100**

Unit-1: Surface Chemistry **[12 hrs]**

Adsorption, adsorption isotherms, Langmuir's unimolecular theory of adsorption statistical derivation of Langmuir's adsorption isotherm, BET theory of multilayer adsorption and its determination

Unit-2: Colloidal state of Matter **[12 hrs]**

Introduction to colloids, classification, properties, specific properties like,electrical properties, charge on colloidal particals, origin of charge, electrical double layer, electrokinetic properties,electrophoresis, electroosmosis, streaming potential, sedimentation potential, determination of size of colloidal particals, applications of colloids, Numericals.

Unit-3: Introduction to Magnetochemistry **[12 hrs]**

Definition of magetic properties, types of magnetic behaviour, sources of paramagnetism, Pascals constants and it's applications, Determination of magnetic susceptibility. Numericals.

Unit-4: Magnetic and Dielectric Properties **[12 hrs]**

Classical theory of diamagnetism, Theory of paramagnetism, Feromagnetism, Molecular filed Theory on ferromagnetism, Below Curie temperature, Domain theory of ferromagnetism, hysteresis of magnetic materials, Anti-ferromagnetic materials, Polarization, Temperature and Frequency effects, electric breakdown, ferroelectric materials, Problems

Unit-5: Magnetic Materials **[12 hrs]**

Atomic magnetism and solids, the exchange interactions, hysteresis loops and their classification, calculation of magnetic moment from saturation magnetization, magnetic domains. Examples of magnetic materials: soft and hard ferrites, i.e. structure and magnetic interactions in spinels, garnets, hexagonal ferrites. Application of magnetic materials

Reference Book

1. K. J. Laidler, J. H. Meiser and B.C. Sanctuary, Physical Chemistry, Houghton Mifflin Company, New York, 2003.
2. A.W. Adamson, Physical Chemistry of Surfaces, 4 th edition, Interscience, New York, 1982.
3. G. K. Vemulapalli, Physical Chemistry, Printice Hall of India.
4. Gurtu and Gurtu , Advanced Physical Chemistry.
5. S.Glasstone, Text book of Physical Chemistry.
6. Gurdeep and Raj, Advanced Physical Chemistry.

7. A.R.West, Solid State Chemistry and its Applications, John Wiley and Sons, 2003(reprint 2009)
8. H.V.Keer, Principles of Solid State.
9. A.Earn Shaw, Introduction to Magnetochemistry, Academic Press.
10. J.Sharma, Magnetochemistry.

CHEP- 418 : Polymer chemistry

04 Hrs/Week Credits: 04 **Marks 100**

Unit-I: Fundamentals of Biological Macromolecules **[12 hrs]**

Chemical bonds in biological systems; Properties of water; Thermodynamic principles in biological systems; Properties and classification of amino acids; Structures of nucleic acids, Protein structure and function, Properties of nucleosides and nucleotides, Composition of nucleic acids, Electrophoresis, Factors affecting on Electrophoretic Mobility; Types of Electrophoresis; Free electrophoresis and Gel electrophoresis; Electrophoresis in genetic analysis; DNA Sequencing and DNA foot Printing.

Unit-II: Macromolecules **[12 hrs]**

Introduction, Formation of synthetic high polymers classification, Polymerization reactions: Chain and Step. Average molecular weight, Number average weight, Methods of determination of molar masses of polymers; Viscosity, Osmometry, Molar mass of charged macromolecules, Donnan membrane equilibrium, Ultracentrifugation, light scattering, Diffusion.

Unit-III: Chemistry of Polymerization **[12 hrs]**

Chain polymerization: free radical polymerization, ionic polymerization, co-ordination polymerization, Ziegler-Natta catalysts. Step Polymerization: polycondensation, polyaddition, ring opening, electro chemical polymerization, group, Transfer polymerization, Polymerization techniques.

Unit-IV: Kinetics of Polymerization **[12 hrs]**

Free radical chain polymerization, Anionic polymerization, Cationic polymerization, Copolymerization, Free radical copolymerization, Ionic copolymerization, Copolycondensation.

Unit-V: Electronically Conducting Polymers **[12 hrs]**

Introduction, Theories of electronic conduction; Band theory of conduction, Hopping conduction, Super conduction, Mechanism of conduction, Doping mechanism, p-type, n-type, auto doping, Stimuli sensitive (smart) polymers, pH and temperature sensitive smart polymers, Applications: Photovoltaic devices, Sensors, LED and Solar cells, Electro chemical devices, Batteries etc.

Reference Book

1. Cantor, C. R. and Schimmel Biophysical Chemistry Vols. 1-3, W. H. Freeman (1980).
2. Lehninger, A.L., Nelson, D. L. and M. M. Lehninger, Principles of Biochemistry 4th Ed., W. H. Freeman (2004).
3. U. Satyanarayana; Biochemistry.
4. Upadhyay; Biophysical Chemistry.
5. L. Stryer, Biochemistry, 5th Edition, (2002) Freeman and Co. New York.
6. D. Voet, J. G. Voet, Biochemistry 3rd Edition (2004), Wiley International Publication.
7. D. L. Nelson and M. M. Cox, Lehninger Principles of Biochemistry 3rd Edition (2002) McMillan North Publication.
8. Polymer Science. By V. R. Gowariker, N. V. Viswnathan, Jayadev Sreedhar.
9. Polymers and Resins. By Brage Golding.
10. Electrical Properties of Polymers. By Tony Blythe and David Bloor.
11. Self doped conducting polymers. By Michael S. Freund and Bhavana Deore.
12. Polymer Science and Technology. By Premamoy Ghosh.

CHEP- 419: Chemical dynamics and catalysis

04 Hrs/Week **Credits: 04** **Marks 100**

Unit-I: Kinetics of Complex Reactions **[12 hrs]**

Opposing or reversible reactions, parallel and competitive reactions, consecutive reactions, chain reactions, branched chain reactions and explosions, hydrogen-oxygen reactions, kinetics of polymerization-step wise and free radical polymerization Effect of temperature on rates of simple and complex reactions. Numericals

Unit-II: Reactions in solution **[12 hrs]**

Diffusion controlled reactions, substitution and correlation effect, Hammet equation, Taft effects, compensation effect. Electron transfer reactions, proton transfer reactions. Ion dipole and dipole-diople interactions. Influence of pressure on rate in solution. Numericals

Unit-III: Photochemical Reactions **[12 hrs]**

Introduction, low of photochemical equivalence, photocatalytic reactions, types of photocatalytic reactions, photooxidation, photoreduction, photosensitization, photocatalytic degradation. Chemiluminescence, photosynthesis. Numericals

Unit-IV: Homogeneous Catalysis **[12 hrs]**

Introduction, mechanism of catalysis, Acid-base catalysis, effect of pH on rate constant. Micellar catalysis, enzyme catalysis, factors governing rate of enzyme reactions, kinetics of enzyme catalysed reactions.Autocatalysis and oscillatory reaction, Lotka-Volterra mechanism, the brusselator, the eregonator, bistability, chemical chaos. Numericals

Unit-V: Surface reactions and Heterogeneous catalysis **[12 hrs]**

Unimolecular surface reactions, bimolecular surface reactions, effect of temperature on heterogeneous reactions, transition state theory and the rates of surface reactions, theory of heterogeneous catalysis, heteropoly acid, general methods for synthesis of hetropolyacid, modification of hetropolyacid, characterization techniques for analysis of hetropolyacid, applications of hetropolyacids.

Reference Books

1. Chemical kinetics- E.S.Laidler pearson Education
   Chemical kinetics and Reaction dynamics -Bul Houston
   Chemical kinetics and Reaction Mechanism -F-Wilkinson-VanNostral Reinhdd

2. kinetics and Mechanism Of Chemical TransformationsJ. Rajaram Macmillan India Ltd J.C.Curiacose.
3. Physical chemistry- Atkin and D.Paula. Oxford University press
4. Physical chemistry- Berry, Rice, Ross Oxford University press
5. Physical chemistry-principles And Appllication in Biological Sciences -Tinoco, Sauer Pearson Education.
6. Physical chemistry-W.J.Moore.

CHEP - 420 (A) : Nanochemistry

04 Hrs/Week **Credits: 04** **Marks 100**

Unit-I: General introduction & synthesis of nanomaterials by physical methods [12Hrs]

Objective of study, synthesis of nanoparticles by physical method, mechanical methods- high energy ball milling, melt mixing, method based on evaporation, physical vapour deposition with consolidation. Ionized cluster beam deposition. Laser vaporization, Laser pyrolysis, sputter diposition, electric arc deposition, Chemical Vapour Deposition (CVD).

Unit-II: Synthesis of Nanomaterials by Chemical Methods [12Hrs]

Introduction, colloids and colloids in solution, interaction of colloids and medium, colloids in vacuum, colloids in medium, effect of charge on colloids, stearic repulsion, synthesis of colloids, growth of nanoparticles, synthesis of metal and semiconductor nanoparticles by colloidal route, Langmuir-Blodgett (L-B) method, sol gel method, electrochemical method.

Unit-III: Analysis Technique [12Hrs]

Introduction, microscopes, electron microscopes,SEM, TEM, Scanning probe microscope (SPM), Scanning Tunnelling microscope, Atomic force microscope, X-ray diffraction, UV-visible and IR spectroscopy.

Unit-IV: Properties, types and application of Nanomaterials [12Hrs]

Properties of nanomaterials – Mechanical, electrical, optical, magnetic, semiconductor.

i. Some special nanomaterials – Carbon nanotubes, porous silicon, Arogels, Zeolites.

ii. Application – Electronic, energy automobiles, sport and toys, textile, cosmetics, domestic appliances, biotechnology, medical, space, defense & environment.

Unit-V: Thin films: [12Hrs]

Introduction, deposition by chemical reactions, deposition by electrochemical reaction, chemical vapor deposition of inorganic Thin films, chemical etching.

Reference Books:

1. Nanotechnology: Principles and practices- Sulabha K. Kulkarni (capital Pub. Co.)
2. NANO- The next revolution –Mohan Surendra Rajan(Natioinal book Trust, India)
3. The British Glass Website- Types of Glass://www.britiglass.org.uk.
4. Fundamental of Nanotechnology – Gabor L. Hornyak, John J. Moore, Harry F. Tibbals, Joydeep Dutta.

5. Recent advances in the liquid phase synthesis of Inorganic Nanoparticles- B. LCushing, V. L. Kolesmichenko & C.J.O".Connor Chemical Review 104, 3893-3946.(2004)
6. Hand book of Thin film technology- H. R. Khan.
7. Thin film phenomenon- K. N. Chopra. Mcgrawa Hill publication
8. Material Science deposition & structure –Milton.

CHEP -420 (B) : Instrumental methods of chemical analysis

04 Hrs/Week Credits: 04 **Marks 100**

Unit-I: General Introduction **[12hrs]**

Overview of Electrode Processes, Electrocapillary curve and electrocapillary maximum potential, exchange current, Ion selective electrodes: Types and construction of electrode, Glass electrode, Solid state electrode and precipitate electrode, Liquid-liquid membrane electrodes, Enzyme and gas electrode, Applications of ion selective electrodes, Reference electrodes, Mercury electrodes (DME, SME, HMDE), numericals.

Unit – II: Potentiometry and Coulometry **[12hrs]**

Potentiometry: Introduction, Instrumentation, Various electrodes in potentiometry:- Ion selective electrode, Liquid membrane electrode, Weston cell. Potentiometric titrations:- Types of potentiometric titrations, Variations in potentiometric titrations, Limitations, Numericals. **Coulometry:** Introduction, Principle, Technique, Coulometry at constant current and coulometry at controlled potential, Coulometric titration, Flowing stream coulometry, Applications, Stripping analysis.

Unit- III: Cyclic Voltammetry **[12hrs]**

Theory and origin of polarography, Interpretation of pornographic curves, Instrumentation of polarography, Differential pulse polarography, Factors affecting on polarographic wave. Introduction and beginning of cyclic voltammetry Range of cyclic voltrametric techniques, Limitations. The acceptable sweep rate range, The shape of the peak in potential sweep curves, The role of non- aqueous solution in cyclic voltammetry, Crieteria of reversibility of electrochemical reactions Quasi reversible and irreversible processes, Qualitative and quantitative analysis by cyclic voltametric techniques, Linear sweep voltammetry for reactions that include simple adsorbed intermediates and Numericals.

Unit-IV: Molecular Luminescence Spectrometry **[12hrs]**

Theory of fluorescence and phosphorescence, Instruments for measuring fluorescence and phosphorescence, Applications and photoluminescence methods, Chemiluminescence.

Unit – V: Thermal methods of analysis **[12 hrs]**

General introduction, classification of thermal methods of analysis thermogravimetry, principles, factors affecting thermal curve, thermogravimetric analysis, Derivative thermogravimetry, Differential thermal analysis - principles, factors affecting DTA curve, applications, differential scanning colorimetry - principles, instrumentation and applications, thermomechanical and dynamic mechanical analysis, thermometric titrations, numericals.

Reference Books:

1. Quantitative analysis -. Alexeyev. V
2. Instrumental methods of analysis – Chatwal and Anand.
3. Introduction to instrumental analysis – R. D. Braun.
4. Instrumental methods of analysis – Willard, Meritt, Dean and Settle.
5. Standard methods of chemical analysis – F. G. Welcher, Vol III, Part A& B.
6. Electroanalytical chemistry – H. W. Neurenberg.
7. Principles of electrochemistry – D. A. Maclines.
8. Ion selective electrodes – (John Wiley) Stulic.
9. Vogel's textbook of quantitative chemical analysis V edition by Jeffery Bassett Mendham Denney.
10. Modern Electrochemistry vol. I - John O'M Bockris
11. Modern Electrochemistry vol. II - John O'M Bockris
12. Analytical Chemistry – Gary D. Christian, 6th edition
13. Principles of Instrumental Analysis–Skoog, F. J. Holler & J. A. Nieman.
14. Instrumental Methods of Chemical Analysis–Galen W. Ewing. 5th edition

CHEP-420 (C) : Advance Quantum chemistry

04 Hrs/Week | Credits: 04 | Marks 100

Unit I: Perturbation Theory: **(12 L)**

Energy and wave-function corrections to wave-function degenerate states, applications including stark effect, hydrogen atom, anharmonic, - quartic oscillators, particle in a box-ground and excited states, time dependent perturbation theory

Unit II: Hartree Fock Theory: **(12 L)**

Slater determinants, Postulate of antisymmetry, Slater- Condon rules for matrix elements, Hartree-Fock equations, Koopman and Brillouin theorems, Roothaan formulation, basis sets, computational aspects, UHF method, Pople Nesbet equations

Unit III: Semi-empirical Theories: **(12 L)**

Recapitulation of Huckel method, extended Huckel method, ZDO approximation, CNDO/INDO methods, Molecular Properties, Computational aspects, MINDO, AM1, PM3 methods, comparison of these methods

Unit IV: Density Functional Theory: **(12 L)**

Introduction, Hohenberg Kohn Theorem, N and V representablity, Levy Functional, Kohn Sham equations, Functional derivatives and local potentials, Thomas Fermi theory, The Kohn-Sham construction, Fractional occupation numbers, Janak's theorem, Slater transition state, Electronegativity, hardness

Unit V: Configuration Interaction: **(12 L)**

Multi-configuration wave function, full CI matrix, doubly excites CI, illustrations, Natural orbitals, Introduction to MC-SCF methods. Truncated CI and size-consistency

Text/Reference Books:

1. Modern Quantum Chemistry, A. Szabo and N.L. Ostlund, Dover, New York (1996)
2. Approximate Molecular Orbital Theory, J. A. Pople and D. L. Beveridge, McGraw Hill, New York (1971)
3. Density Functional Theory of Atoms and Molecules, R. G. Parr and W. Yang, Oxford University Press, Oxford (1989)
4. Molecular Modeling, A. Leach, Longman, Landon (1996)

CHEP- 421 : Laboratory course

4.5 Hrs/Week **Credits: 04** **Marks 50**

Spectroscopy

1) To determine the indicator constant pK_{in} of an indicator by using half height method (Bromo cresol purple)
2) To determine the concentration of Fe(II) and Cu(II) by spectrophotometric titration with EDTA.
3) To investigate the reaction kinetics between $K_2S_2O_8$ and KI by spectrophotometrically
4) To determine simultaneously the dichromate and permanganate ions in the given solution.

Polarimetry

5) Determine the percentage of two optically active substances in a mixture.
6) To investigate the complex ion formation between Fe(II) and thiocynate ion.
7) Investigate the effect of substitution of chloride ions on rate constant of inversion of cane sugar by using mono, di and trichloro acetic acid as catalyst.

Refractometry

8) Determine the refractive indices of series of solution of a salt and determine the concentration of the salt in the given unknown solution.
9) Study the variation of refractive indices with composition of mixture of carbon tetrachloride and ethyl acetate and determine the composition and molar refraction of the given unknown mixture.

Viscosity

10) Determine the variation of viscosity with composition of I) ethanol-water, II) methanol-ethylidene chloride, III) nitric acid- chloroform and and conform the formation of compound.
11) Determine the molecular weight of macromolecules.

Flame Photometry

12) Estimation of Na, K, Li & Ca by flame photometry.

Chemical Dynamics

13) Investigate the influence of ionic strength on the rate constant of the reaction between $K_2S_2O_8$ and KI.
14) Determine the order of a reaction by 1) substitution method, (II) fractional change method and (III) differential method.
15) Investigate the reaction between bromic acid and hydrochloric acid.
16) Investigate the kinetics of iodination of acetone.

Phase equalibria

17) Determine the critical solution temperature of phenol and water in presence of 1) 1% NaCl 2) 0.5% naphthalene 3) succinic acid
18) Construct the phase diagram of three-component system containing ethanol benzene and water.
19) Determine the equilibrium constant of the tri-iodide formation in aqueous solution by distribution method.
20) Determine the formula of the complex formed between cupric ion and ammonia by distribution method.

Reference Book

1. Systematic experimental physical chemistry – S.W. Rajbhoj & T. K. Chondhekar
2. Experiments in chemistry – D.V. Jahagirdar

CHEP- 422 : Laboratory course

4.5 Hrs/Week **Credits: 04** **Marks 50**

Potentiometer

1) Titrate ferrous ammonium sulphate with cerric sulphate and find out formal redox potential of Fe^{+2}/Fe^{+3} and Ce^{+3}/Ce^{+4} system
2) Titrate potentiometrically phosphoric acid solution against NaOH and calculate pK_1, pK_2 and pK_3 of the acid.
3) To determine the standard free energy changes ΔG° and equilibrium constant for reaction $Cu + 2Ag^+ \longrightarrow Cu^{++} + Ag$ (TKC-167)
4) Determine the activity coefficient of silver ions using a concentration cell without transference.

pH metry

5) To determine the proton-ligand stability constant of an organic acid and the metal-ligand stability constant of its complex by pH measurements.
6) Determine the Hammett constant of a given substituted benzoic acid by pH measurements.
7) Determine the pH values of various mixtures of sodium acetate and acetic acid in aqueous solution and hence find out the dissociation constant of the acid.
8) To determine the hydrolysis constant of aniline hydrochloride by pH measurements.

Conductometry

9) Conductometric titration of a mixture of strong acid, weak acid and a salt.
10) To determine the degree of hydrolysis and hydrolysis constant of sodium acetate conductometrically.
11) Determine the amount of trichloroacetic acid, monoacetic acid and acetic acid in a given solution by conductometric titration against sodium hydroxide solution.

Magnetochemistry

12) To determine the magnetic susceptibility and number of unpaired electrons in given compound.
13) Verification of Weidemann's law using nickel chloride solution.

Surface Tension

14) Study the effect of surfactant (n-propyl alcohol) at various concentrations on the surface tension of water and hence determine the limiting cross sectional area of alcohol molecule by stalagmometer.
15) To study the effect of surfactant on surface tension of water by parachor of a solid by stalagmometer.

Adsorption

16) Investigate the adsorption of acetic / oxalic acid by activated charcoal and test the validity of Freundlich and Langmuir's isotherm.

Thermodynamics

17) Determine the partial molar volume of ethanol and water in a given composition by density measurements.
18) To determine heat of neutralization of strong acid and heat of ionization of weak acid calorimetrically.
19) To determine the integral heat of solution of KNO_3.

Reference Book

3. Systematic experimental physical chemistry - S.W. Rajbhoj &T. K. Chondhekar
4. Experiments in chemistry – D.V. Jahagirdar

CHEP - 423 : Research project (Experimental)

4.5 Hrs/Week **Credit : 4.5** **50 Marks**

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CHEP- 424 : Research project (Dissertation, presentation and Seminars)

4.5 Hrs/week **Credit : 4.5** **50 Marks**

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Dean
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