SWAMI RAMANAND TEERTH MARATHWADA UNIVERSITY, NANDED

M.Sc. PHYSICAL CHEMISTRY Second Year

(SEMISTER III & IV)

CBCS Pattern

June 2015

Semester	Paper	Course No.	Course	Periods / week	Total Periods	Marks
III Semester	XV	CH-531	Advanced Spectroscopic Methods	4	60	4 Credits
	XVI	CH-532/3	Solid State Chemistry	4	60	4 Credits
	XVII	CH-533/3	Chemical Dynamics	4	60	4 Credits
	XVIII	CH-534/3	Elective Paper A. Statistical Thermodynamics B. Advanced Quantum Chemistry	4	60	4 Credits
	XIX		Seminar			1 Credit
IV Semester	XX	CH-541/3	Radiation Chemistry	4	60	4 Credit
	XXI	CH-542/3	Photochemistry	4	60	4 Credit
	XXII	CH-543/3	Molecular Reaction Dynamics & Bio Physical Chemistry	4	60	4 Credit
	XXIII	CH-544/3	Elective Paper A. Electrochemistry B. Liquid State	4	60	4 Credit
	XXIV		Seminar			1 Credit
Lab Course Annual	XXV	CH-501/3	Lab course V	6	132	4 Credit
	XXVI	CH-502/3	Lab Course VI	6	132	4 Credit
	XXVII	CH-503/3	Lab Course VII	6	132	4 Credit
	XXVIII	CH-504/3	Lab Course VIII	6	132	4 Credit

Note : 1) Each Laboratory Course of 6 Hrs duration should be completed in 6 Hrs per day.

2) Each student has to give one Seminar in each semester (2.50 Marks). The marks to be given in fourth semester (Internal Marks 25)

3) Research oriented project to be completed in 12 hrs per week (6hrs per day) having 100 marks. The assessment of project is done by external Examiner at the time practical examination

M Sc Part-II Year Examination Physical Chemistry
(Semester Pattern)

Semester	Paper	Course No	Course	Periods/ Week	Total periods	Credit
III	XV	CH-531	Advanced spectroscopy methods	04	60	4
	XVI	CH-532/3	Solid State Chemistry	04	60	4
	XVII	CH-533/3	Chemical Dynamics	04	60	4
	XVIII	CH-534/3	Elective: a)Statistical Thermodynamics b)Advanced quantum chemistry	04	60	4
	XIX		Seminar			1
IV	XX	CH-541/3	Radiation Chemistry	04	60	4
	XXI	CH-542/3	Photochemistry	04	60	4
	XXII	CH-543/3	Molecular Dynamics& Bio physical chemistry	04	60	4
	XXIII	CH-544/3	Elective :a)Electrochemistry b)Liquid state	04	60	4
	XXIV		Seminar			1
Lab course Annual pattern	XXV	CH-501/3	Lab course V	6	132	4
	XXVI	CH-502/3	Lab course VI	6	132	4
	XXVII	CH-503/3	Lab course VII	6	132	4
	XXVIII	CH-504/3	Lab course VIII	6	132	4

Draft Syllabus Prescribed For

M Sc Part-II Year Examination Physical Chemistry
(Semester Pattern)

Semester	Paper	Course No	External (ESE)	Internal (CA)	Total
III	XV	CH-531	75 marks	25 marks.[2 tests:15 marks+Assignment:10 marks]	Credits 4 100 marks
	XVI	CH-532/3	75 marks	25 marks.[2 tests:15 marks+Assignment:10 marks	Credits 4 100 marks
	XVII	CH-533/3	75 marks	25 marks.[2 tests:15 marks+Assignment:10 marks	Credits 4 100 marks
	XVIII	CH-534/3	75 marks	25 marks.[2 tests:15 marks+Assignment:10 marks	Credits 4 100 marks
	XIX	Seminar	25 Marks		Credit 1
IV	XX	CH-541/3	75 marks	25 marks.[2 tests:15 marks+Assignment:10 marks]	Credits 4 100 marks
	XXI	CH-542/3	75 marks	25 marks. [2tests:15marks+Assignment:10 marks]	Credits 4 100 marks
	XXII	CH-543/3	75 marks	25 marks. [2tests:15marks+Assignment:10 marks]	Credits 4 100 marks
	XXIII	CH-544/3	75 marks	25 marks [2tests:15marks+Assignment:10 marks]	Credits 4 100 marks
	XXIV	Seminar	25 Marks	---	Credit 1
Lab course Annual pattern	XXV	CH-501/3	75 marks	25 marks [2tests:15marks+Assignment:10 marks]	Credits 4 100 marks
	XXVI	CH-502/3	75 marks	25 marks [2tests:15marks+Assignment:10 marks]	Credits 4 100 marks
	XXVII	CH-503/3	75 marks	25 marks [2tests:15marks+Assignment:10 marks]	Credits 4 100 marks
	XXVIII	CH-504/3	75 marks	25 marks	Credits 4 100 marks

M. Sc. Second Year, Semester-III
Paper–XV, [CH-531]
Advanced Spectroscopic Methods

Marks: 4 Credit **Periods: 60**

SM-1: UV-Vis Spectroscopy:
SM-2: IR spectroscopy:
SM-3: NMR Spectroscopy (Organic):
SM-4: NMR Spectroscopy (Inorganic):
SM-5: Mass Spectroscopy:
SM-6: Moissabaur Spectroscopy:
SM-7: Structural problems:

SM-1: UV-Vis Spectroscopy: **06P**

Fieser-Woodward rules for conjugated dienes and carbonyl compounds, Fieser-Kuhn rules for polyenes. UV spectra of aromatic compounds and heteroaromatic compounds. Calculation of $\cdot_{max}$ for the benzene derivatives ($R\text{-}C_6H_4\text{-}Co\text{-}G$) by A. I. Scott emperical rules.

SM-2: IR spectroscopy: **10P**

a) Recapitulation, Characteristic vibration frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds Ketones, aldehydes, esters, amides, acids, anhydride, Lactose, lactams and conjugated carbonyl compounds. Factors affecting group frequencies: overtones, combination bands and Fermi-resonance. FITR and sampling technique.

b) Structural information from vibrational spectra: Group frequencies, Characteristic band stretching frequencies, Mode of vibrations of linear and non-linear molecules, deformation, frequencies of carbonyl metal complexes, pattern of group frequencies, mode of bonding of ambidentate ligands, Cynides, Ethylenediamine and Diketone complexes.

SM-3: NMR Spectroscopy (Organic): **12P**

a) $_1$H NMR: General introduction and definations, Chemical shift, Spin-spininteraction, shielding mechanism of measurement of chemical shift values andcorrelation for protons bonded to carbon (aliphatic, olefinic, aldehyde andaromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines,amides and mercapto). Factors affecting chemical shift. Deuterium exchange.Spin-spin coupling, factors affecting coupling constant. Complex spin-spininteraction between two and three nuclei. Simplification of complex spectra,nuclear magnetic double resonance, contact shift reagents, solvent effects. Fouriertransform technique. Nuclear Over-Hauser effect (NOE). Resonance of other nuclei; $_{19}$F and $_{31}$P.

b) $_{13}$C NMR: Resolution and multiplicity of $_{13}$C NMR, 1H-decoupling, noise decoupling, broad band decoupling; Deuterium, fluorine and phosphorus coupling; NOE signal enhancement, off-resonance, proton decoupling, Structural applications of CMR. DEPT; Introduction to 2D-NMR: COSY, NOESY, DEPT, INPET, APT, INADEQUATE.

SM-4: NMR Spectroscopy (Inorganic): **08P**

a) Basic principle of NMR spectroscopy and applications to Paramagnetic compounds and metal nuclei of Pt $_{195}$ and Sn $_{119}$.

b) Basic principle and applications of ESR spectroscopy to different free radical molecules and transition metal ion complexes.

SM-5: Mass Spectroscopy: **06P**

Theory, instrumentation and modifications; Unit mass and molecular ions; Important terms- singly and doubly charged ions, metastable peak, base peak, isotropic mass peaks, relative intensity, FTMS, etc.; Recognition of M+ ion peak; Generalfragmentation rules: Fragmentation of various classes of organic molecules, including compounds containing oxygen, sulphur, nitrogen and halogens; α-, β-, allylic andbenzylic cleavage; McLafferty rearrangement.

SM-6: Moissabaur Spectroscopy: 08P

Basic priniciple of Moissabaur Spectroscopy, applications on the basis of isomer shifts, electric quadrupole interactions. Elucidation of structure of $I_2Br_2Cl_4$, I_2Cl_6, Fe^{+2} and Fe^{+3} complexes and Sn^{+2} and Sn^{+4} compounds

SM-7: Structural problems: 10P

a) Combined problems on UV, IR, NMR and Mass spectral data for structure determination.
b) Elucidition of structure of organic molecules using spectra (IR & NMR).

Reference Books:

1. Spectroscopic identification of Organic Compounds, R. M. Silverstern, G. C. Bassler and T. C. Morril.
2. Introduction to NMR spectroscopy, R. J. Abraham, J. Fisher and P. Loftus.
3. Application of spectroscopy of organic compounds – J. R. Dyer.
4. Spectroscopy of organic compounds, P. S. Kalsi.
5. Organic Spectroscopy, William Kamp.
6. Organic Chemistry, R. T. Morrison and R. N. Boyd.
7. Practical NMR spectroscopy, M. L. Martin, J. J. Delpench and G. J. Martin.
8. Spectroscopic methods in organic Chemistry, D. H. William, I. Fleming.
9. Fundamentals of Molecular spectroscopy – C.N.Banwel

M. Sc. Second Year, Semester-III
Paper–XVI, [CH-532/3]
Solid State Chemistry

Marks: 4 Credit **Periods: 60**

1. Solid State reactions **08P**

General Principles, experimental procedures, co-precipitation as precursor to solid state reactions, kinetics of solid state reactions.

2. Crystal Defects and Non-Stoichiometry **14P**

Perfect and imperfect crystals, instrinsic and extrinsic defects – point defects, line and plane defects, vacancies-Schottky defects and Frenkel defects. Thermodyamics of Schottky and Frenkel defect formation colour centres, non-stocichiometry and defects.

3. Electronic Properties and Band Theory **24P**

Metals, insulators and semiconductors, electronic structure of solids band theory, band structure of metals, insulators and semiconductors, intrinic and extrnisic semiconductors, doping semiconductors, p-n junctions, super conductors,
Optical properties–optical reflectance, phorotconduction–photoelectric effects.
Magnetic properties – classification of materials : quantum theory of paramagneticscooperative phenomena – magnetic domains hysteresius.

4. Organic solids **14P**

Electrically conducting solids, organic charge transfer comlex, organic metals, new superconductors.

Books Referred

1. Solid State Chemistry adn its Applications, A.R. West Plenum
2. Principles of the Solid State, H.V. Keer, Wiley Eastern
3. Solid State Chemistry N.B. Hannay
4. Solid State Chemisty D.K. Chakarabarty, New Age International

M. Sc. Second Year, Semester-III
Paper–XVII, [CH-533/3]
Chemical Dnyamics

Marks: 4 Credit **Periods: 60**

1. Molecules in Motion **14P**

a. Molecular motion in gases : collision with walls and surface rate of effusion, migration down gradients, transport properties of a perfect gas.

b. Motion in liquids : Structure of liquids, molecular motion in liquids conductivites of electrolyte solution, mobilities of ions conductivtes and ion-ion interactions.

c. Diffusion : a Thermodynamic view, the diffusion equation, diffusion probabilities statistical veiw. Problems on every concept.

2. Rate of chemical Reactions **08P**

Experimental techniques rates of reactions, integrated rate laws, reactions approacting equilibrium, temperature dependence of reaction rates. According for the rate laws. Elementary reactions, consecutive elementary reactions, unimolecular reactions.Problems.

3. Kinetics of Complex reactions: **19P**

a. Chain reactions : Structure of chain reactions, Explosions, photochemical reactions.

b. Polymerisation Kinetics : Chain Polymerisation, stepwise Polymerisation

c. Catalysis and oscillations : Homogenous catalysis, autocataysis, oscillatingreactions, chemical chaos. Problems.

4. Molecular Reaction Dynamics : **19P**

a. Reactive encounters : Collision theory, diffusion controlled reactions.

b. Activated complex theory : The reactions coordinate and transition state, Erying equation, thermodynamic aspects of activated complex theory.

c. Dynamics of Molecular collisions : reactive collisions, Potential energy surfaces. Problems.

Books Suggested :

1. Physical Chemistry, P.W. Atkins (ELBS)
2. Chemiscal Kinetics, K.J. Laidler, Tatamacgraw Hill Publishing Co. Lted., News Delhi.
3. Reaction Mechanism and chemical Transformations, J. Rajaram and K. Kuriakose.

M. Sc. Second Year, Semester-III
Paper–XVIII, [CH-534/3A]
Statistical Thermodynamics

Marks: 4 Credit **Periods: 60**

1. Background concepts 08P

Combinatorial problems, number ways in whcih particles can be arranged in order or placed in container. The situations of this distribution in Bolltzman, Fermi-Direac andBose Einstein statistics, illustrations stirling approxmation, Langrange method ofUndetermined multiipliers, distribution and most probable distribution. Problems.

2. Statistical Mechanics of a System of Independent Particles 10P

Introduction : distribution laws, partition functions and its significance, limit of aplicability of various distribution laws, Relation between partition function and thermodynamics function, illustrative examples and problems.

3. Types of Statstics 08P

Maxweel – Boltzmann statistics, Fermi-Dirac statistics and Bose-Einstein statistics

4. Application of Statistical Mechancics 18P

a. Ideal gases : Partition function of a monoatomic gas. Thermodynamics function of a monoatomic gas, diatomic and polyatomic gases. Internal rotation of a polyatomic molecule, heat capacity and the residual entropies of polyatomic molecules.

b. Solids : Introduction, Thermal characteristics of crystalline solids. Einstein model, Debye modification, limitiations and modifications of Debye theory and comparision between debye theory and Einstein model.

c. Solutions : Introduction, lattice modals, Ideal solution, non-ideal soluitons, polymer solutions.

5. Nuclear spin Statistics : 10P

Introduction, the mean symmetry and the nuclear spin, ortho and para nuclear states, ortho, and para hydrgen, nulcear spin stratistics of deuterium

6. Fluctuations : 06P

Introduction, the mean distribution and mean square deviation, fluctutaion in energy in a canonical ensesmble, fluctuations in density and radioactive disintegrations, The Brownian movement. Problems.

Book Suggested :

1. Statistical Thermodynamics, Donald A. Mc Quarrie, Happer and Row, New York,1973.
2. Statistical Thermodynmics, M.C. Gupta, Wileyt Eastern Limited. New Delhi,1990
3. Elements of Statistical Thermodynamics, L.K. Nash, Addison Wesley, MenloPark, 1992.
4. Text book of Pohysical Chemistry, Samuel M. Glastone, Littern EducationalPublishing In., New York.
5. Physical Chemistry, P.W. Atkins (ELBS)

M. Sc. Second Year, Semester-III
Paper–XVII, [CH-534/3B]
Advanced Quantum Chemistry

Marks: 4 Credit **Periods: 60**

(Pre-requisite Methematics at least up to five year B.Sc. Level is necessary. At least one PC among 4 students should be available)

1. Theoretical and Computational Treatment of Atoms and Molecules, Hartee-Fock Theory. **16P**

Review of the principles of quantum mechanics, Born-Oppenheimer approximation. Slater-condon rule. Hartree-Fock equation, Koopmans and Brillouin theories, Roothan equation, Gaussion basis sets.

2. Confirguration Interaction and MC-SCF **16P**

Introduction to Cl; full and truncated Cl theorties, size consistency. Introductorytreatment of coupled cluster and MC-SCF methods.

3. Semi – emerical theories **16P**

A review of the huckel, EHT and PPP treatments ZDO approximation detailedtreatment of CNDO and INDO theories. A discussion of electronic energies andproperties. An Introduction to MOPAC and ANI with hands on eperience on personalcomputers

4. Density functional theory **12P**

Derivation of Hohenberg – Kohn theorem, Kohn – Sham formulation, N and V representabilities, review of the performance of the exiting local (e.g-slater Xa and other methods) and non-local functionals treatment of chemical concepts with the density functional theory

\Book Referred

1. modern quantum chemistry N.S. ostlund and A. Szabo Mcgrall hill.
2. Methods of molecular quamtum mecheanics R. McWeeny and B.T. sSutcliffe.Academics press.
3. Density functional theory of Atoms and Molecules R.G Parr and W.yang Oxford
4. Exploring Chemistry with electron structure methods J.B. Foresman and E. FrishFoussian Inc

M. Sc. Second Year, Semester-IV
Paper–XX, [CH-541/3]
Radiation Chemistry

Marks: 4 Credit **Periods: 60**

1. Radioactivity : **11P**

Historical background, natural radioactive elements, general characteristics of α, β, γ rays, detection and measurement of radioactivity, the theory of radioactive disintegration, decay kinetics, units of radioactivity parent daughter growth relationship secular and transient equilibrium, theory of α decay, β decay – energetics of β decay, problems of β decay, Fermi's theory of β decay, nuclear deexcitation emission, Numerical.

2. Nuclear Reactions and Reactors : **16P**

Definition and Bethes notation, nuclear reaction energetics, nuclear reaction and threshold energy, characteristics of nuclear reactions, types of nuclear reactions, conservation in nuclear reactions, specific nuclear reactions- photoncluear reactions, stripping and pickup reactions, evaporation, spallation, fragmentation, direct nuclear reactions, thermonuclear reactions.

Fission energy, natural uranium reactor, four factor formula, classifications of nuclear reactors, reactor power, critical size of thermal reactor, breeder reactor, India's nuclear energy programme, nuclear waste management, energy from nuclear fission. Numerical

3. Elements of Radiation Chemistry : **13P**

Introduction: Primary effects due to charged particle/radiation, Linear energy transfer (LET), interactions of electron with matter, interaction of neutrons with matter, interaction of heavy charged particles with matter, interaction of rays with matter, units for measuring radiation absorption, absorption in water.

Radiation dosimeter-units of radiation energy, Chemical dosimeter- the Fricke dosimeter, ceric sulphate dosimeter, other chemical dosimeters conversions of measured dose values. Numerical

4. Effects of Radiation on Matter: **11P**

Radiolysis of water and aqueous solutions. Radiolysis of water vapour, liquid water. Radiolysis of oxygenized water. The reduced species-hydrated electrons. Redox reactions due to ray irradiated, radiation induced colour centers in crystals (strong and release of energy), effect of pH on radiolytic product of water solution, Radiolysis of aqueous solution : Radiolysis of ferric solution, ferrous sulphate, cupric sulphate solution, Radiolysis of aqueous solution of organic compounds Numerical

5. Application of radioactivity: **09P**

Typical reactions involved in the preparations of isotopes : the scillard-chalmers reactions, radiochemical principles in the use of tracers, typical application of radioisotopes as tracers-chemical investigation, physio-chemical research, analytical applications, agricultural applications, industrial applications, use of nuclear radiations, radioisotope as a source of electricity.

Reference Books :

1. Source of atomic energy by s. Glasstone, D. Van Nostrated co. INC
2. Essentials of Nuclear Chemistry by H.J. Arnikar 4th Edn, New Age Inter. (p) Ltd.
3. Introduction to Nuclear Chemistry by B.G. Harvey.
4. Nuclear Chemistry by M.G. Arora & M. Singh Anmol publication, New Delhi.
5. Elements of Nuclear Chemistry by A.K. Srivastav, P.C. Jain, S. Chand & Co.
6. A text book of Nuclear Chemistry by C.V. Shekar Deminat publication & distribution, New Delhi.
7. Radiochemistry & Nuclear Chemistry, 3rd edn G. chappin, Butterwerth-Heinemann.

M. Sc. Second Year, Semester-IV
Paper–XXI, [CH-542/3]
Photochemistry

Marks: 4 Credit **Periods: 60**

1. Photochemical Reactions **06P**

Interaction of electromagnetic radiation with matter, types of excitation, rate of excited molecule, quantum yield, transfer of excitation energy, actionomety.

2. Determination of Reaction Mechanism **06P**

Classification, rate constrant and life times of reactive energy states determination of rate constrats of reactions, effects of light intensity on the rate of photochemicls reactions, types of photochemical reactions – photo-dissociation, gas phase photoysis.

3. Photophysical process in electronically excited molecules **14P**

Types of photochemistry, pathways with Jabalonski diagram Radiation – Theory, Internal Conversion and intersystem crossing.
Fluorescence emission
Fluorescence and structure
Triplet states and phosophorescence emission
Emission property and the electronic configuration
Photophysical kinetics of unimolecular process
State diagrams Delayed fluorescence
The effect of temperature on emission process

4. Photophyscial kinetics of Biomolecular Process **13P**

Kinetic collisions and optical collision
Biomolecular collisions in gases and vapours and the mechanism of Fluorescence quenching
Collisions in solution
Kinetics of collissions quenching, stern-Volmer equation
Concentration dependance of quenching and excimer formation
Quenching by foreign subsdtances.

5. Some aspects of organic and Inorganic photochemistry **13P**

Photoreduction and reactions
Photoxidation and photooxygenation
Cycloaddition reactions
Woodward – Hoffman rule of electrocyclic reactions
Chemiluminescence
Transition mental complexes

6. Some current Topics in photochemistry **08P**

Photosynthesis
Photoelectrochemistry of excites state redox reaction
Solar energy conversion and storage

Book Referred

1. Fundamentals of Photochemistry, K.K. Rohtagi-Mukherji, Wileyeastern
2. Essentials of Molecular Photochemistry a. Giolber and J. Baggot, Black well Scientific Publication
3. Molecular Photochemisty, N.J. Turro, W.A. Benjamin
4. Introductory Photochemistry, A. Cox and T. Camp. Mcgraw-Hill
5. Photochemistry R.P. Kundall and A. Gilbert, Thomson Nelson
6. Organic Photochemistry, J. Coxon and B. Halton, Camnridge University Press

M. Sc. Second Year, Semester-IV
Paper–XXII, [CH-543/3]
Molecular Reaction Dynamics and Biophysical Chemistry

Marks: 4 Credit **Periods: 60**

1. Molecular Reaction Dynamics **20P**

a. Reactive encounters : Collision theory, diffusion controlled reactions.
b. Activated complex theory : The reaction coordinate and transition state, Erying equation, thermodynamic aspects of activated complex theory.
c. Dynamics of Molecular collisions : reactive collisions, Potential energy surfaces. Problems.

2. Biophysical Chemistry

1. Biological Cell and its Constitents **03P**

Biological cell structure and functions of proteins, enzymes DNA and RNA in living systems. Helix coll trastion.

2. Bioenergetics 04P

Stadard free energy change in biochemical reactions, exergonic, endergonic, Hydrolysis of ATP, synthesis of ATP from ADP

3. Statistical Mechanics in Bioploymers **06P**

Chian configuration of macromolecules, statistical distribution end to end dimensions, calculation of average dimensioin of vairous chain stuctures, polypeptide and protein structures, introduction to protein folding problem.

4. Biopolymer Interactions **07P**

Forces involved in biopolymer interactions.electrostatic charges and molecular expansion, hydrophobic forces, dispersion force interactions. Multiple equilibria and various types of binding processes in biological systems. Hydrogen ion titration curyes.

5. Thermodynamics of Biopolymer solutions. **06P**

Thermodyamics of biopolymer solutions, osmotic pressure, membrane equilibrium muscular contraction and energy genaration in mechanoichemical system.

6. Cell Membrane and Transport of lons **04P**

Structure and functions of cell membrane, ion transport through cell meembrane, irreversible thermodynamic treatment of membrane transport. Nerve conduction.

7. Biopolymers and their molecular Weights **06P**

Evalution of size, shape, molecular Weight and expect of hydration of Biopolyment by various experimental techniques. Sedimentation equilibrium, hydrodynamic methods, diffusion, sedimention velocity, viscosity, electrophoresis and rotional motions.

8. Diffraction Methods **04P**

Light scattering, low angle X-ray scattering, X-ray diffraction and photo corrleation spectroscopy, ORD

Book Suggested :

1. Principles opf BioChemistry A.L.Lehniger, Worth Publisher
2. Biochemistry, L. Stryer, W.H. Freeman
3. Biochemistry, J. Devidrawn, Neil Patterson
4. Biochemistry, Voet, Jphn Wiley
5. Qutines of Biochemisty E.E. Conn and P.K. Stumpf, Jojn Wiley
6. Bioinorganic Chemistry, A Chemical Approch to Enzyme Action, H. Dugas and C. Penny, Springer-Vertag.
7. Macromolecules structure and function F. Would, Prentice Hall

M. Sc. Second Year, Semester-IV
Paper–XXIII, [CH-544/3A]
Electrochemistry

Marks: 4 Credit **Periods: 60**

1. Introduction **08P**

Basic Introduction to eletrolytic conductance, theory of electrolytic dissociation, mechanism of electrolytic conductance and the migration of ions. Problems.

2. Free Energy and Activity **19P**

Activity and activity coefficient, equilibrium and free energy changes, Debye-Huckel theory, Debye-Huckel limiting law, Debye-Huckel equation of appreciable concentration, Huckel and Bronsted equation, quantitative verification of appreciable concentrtions, Huckel and Bronsted equation, quantitative verification of Debye-Huckel equation, tests, of DebyeHuckel limiting equation, activities in concentration solutions.,extension of Debye-Huckel theory, ion association, equilibria in electrolytes, strong intermaediates and weak electorlytes, soulubility, solubility product principle, soulubility for common ions and complexion, determination of instability constant, activity coefficient form soulubility, measurements solubility and Deye-Huckel theory. Problems

3. Reversible Cells **19P**

a. Reversible and irreversible cells, reversible electrodes, application or emf measurements, concentration cells with a single electrolyte., amalgam concentration cells, electrode potential, potentials in nonaqueous soultions, factors affecting electrode potentails, rate or relectrode potentials, electrode potentials and wquilibruim constants, electrode potentials and soulbility proucts.

b. Oxidation reduction syste: types of oxidations reduction systems, determination of oxidation reduction potentials. Problems.

4. Dyanmic Electrochemistry : **14P**

Process at electrodes., electrical double layer, rate of charge transfer, polarisation, electrochemical process, electrolysis, characteristics of working eclls,. Power production and corrosion, types of electrochemical corrosions, fuel cells, powere generation in fule cells, power storage, secondary cells, thermodynamics and kinetics of corrsion and their prevention methods, applications of electrolysis in electrorefining, electroplating and electrotyping. Problems.

Books Suggested :

1. Text book of Physical Chemistry, Samuel. M.Glastone, Littern Educational publishing in., New York
2. Physical Chemeistry, P.W.Atkins (ELBS)
3. Introduction to electrochemistry, Samuel M. Glastone, Littern Educational. Publishing inc., New Yourl.
4. Theoritical electrochemistry, L. J. Antropov., Mir Publioshers, Moscow
5. Modern electrochemistry vol I & II Bokris J.O.M. and Reddy A.K.M (pLENUM)

M. Sc. Second Year, Semester-IV
Paper–XXIII, [CH-544/3B]
Electrochemistry

Marks: 4 Credit **Periods: 60**

1. General properties of liquids **15P**

a) Liquids as dense gases, liquids as disordered solids, some thermodynamic relations, internal pressure and its significance in liquids. Equations of state, critical constants. Different types of intermolecular forces in liquids, different potentialfunction for liquids, additivity of pair potential approximation.

b) A classical partition function for liquds, correspondence principle,configuration integral, configuration properties.

2. Theory of Liquids. **14P**

Theory of liquids, partition function method or model approach; single cell models, communal energy and entropy LTD model, significant structure model.

3. Distribution Function and Related Equations **18P**

Radial distribution function method, equation of state ion terms of RDF, Molecular distribution functions, pair distribution function, relationship between pair distribution function and pair potential function. The IBG equation, the HNC equation, the PY equation, cluster expansion.

4. Methods for structure Determination and computational Techniques. **13P**

Spectroscopic techniqes for liquid dyanamic structure studies, Neutron and X-ray scattering spectroscopy Computation Techniques- Monte Carlo and molecular dynamics methods.,

Books Referred :-

1. An introudction to Liquid state P.A. Egelstaff, Academic Press
2. The Dynamic Liquid State, A.F.M. Bartion, Longman.
3. The Liquid State, J.A. Pryde
4. Significant Liquid Structures, H.Eyring and M.S. John.

M. Sc. Second Year
Laboratory Course-V,
Paper– XV, CH-501

Marks: 4 Credit **Periods: 132**

Spectroscopy

1) To determine the indicator constant $P_{K^{IN}}$ of and indicator by using half height method (Bromo cresol purple) (DVJ-200)
2) To determine the stability constant of metal complex between 5-SSA and Fe +3 with the help of job's curve and Bent and French method (for weak complex) (dvJ204)
3) To determine the concentration of Fe (II) and Cu (II) by soectrophotmetric titration with EDTA
4) To investigate the effect of ionic strength on pKa of bromo cresol green and thus determine pk_{in} (DVJ-211)
5) To invistigate the reaction kineties between $K_2S_2O_8$ and KI by spectrophotometry (TKC-223)
6) To determine simultaneously the dichromate and permanganate ions in the given soulution

POLARIMETRY

7) Determine the percentage of two optically active substances in a mixture (TKC-194)
8) To investigate the complex ion formation between Fe (II) and thiocyanate ion
9) To study Kinetics of hydrolysis of sucrose by Hammett-Zuckerman approach (DVJ)
10) Investigate the effect of substitution of chloride ions on rate constan of inversion of cane sugar by using mono, di, and trichlore acetic acid as catalyst

REFRACTOMETRY

11) Determine the refractive indices of series of solution of a salt and determine the concentration of the salt in the given unknown solution.
12) Determine the molar refration of ethyl, prooyl and butly acetate and show the constancy of contribution to the molar refraction amde by CH2 group
13) Determine the molar refration of methyl acetate, ethyl acetate, n-hexane and carbon tetrachloride and calculate the atomic refraction of C, H and Cl atoms.
14) Study the variation of refractive index with composition of mixtures of carbon tetrachloride and ethyl aetate and determine the molar refraction of the givenunknown mixture.

VISCOSITY

15) Study the variation of viscosity with composition of 1) ethanol – water II) methanol – ethylidene chloride III) the formation of compound (TKC 25)
16) Determine the molecular weight of macromolecules (TKC 251)
17) Determine the iso-electric point of gelation and examine the effect of aging by viscometric methods (DVJ-29)

FLAME PHOTOMETRY

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

M. Sc. Second Year
Laboratory Course-VI,
Paper– XXVI, CH-502

Marks: 4 Credit **Periods: 132**

Potentiometer

1) Titrate ferrous ammonium sulphate with cerric sulophate and find out formal redox potential of $Re^{2+/}Fe^{3+}$ and Ce $^{3+}/Ce^{4+}$ system

2) Titrate potentionmetriaclly phosphoric acid solution against NaOH and calculate Pk_1, Pk_2 and Pk_3 of the acid

3) Titrate potentiometrically NaCl soulution against AgNO3 and find out the concentration of NaCl and hence determine the solubility product of AgCl

4) To determine the standad free energy change ^G0 and equilibrium constant for the reaction. Cu + 2Ag+ ------· Cu^{++} + Ag (TKC-167)

5) Determine the activity coefficient of sivlver ions using a concentration cell without transference (TKC-154)

$_P$H METRY

6) To determine the product lignd stability constant of an organic acid and the metal ligand stability constant of its complex by pH measurements (TKC-176)

7) Determine the Hammett constant of a given substituted benzoic acid by pH measurements (TKC-170)

8) Determine the pH valuse of various mixtures of sodium acetate and acetic acid in aqueous solution and hence find out the dissociation constant of the acid (TKC-173)

9) To determine the hydrolysis constant of aniline hydrochloride by pH measurements (TKC-174)

Conductometry

10) To determine the thermodynamic dissociation constant of weak acid conductometrically.

11) Investigate the kinetics of basic hydrolysis of ethyl acetate conductometrically.

12) Conductometric titration of a mixture of strong acid weak acid and a salt (DVJ)

13) To determine the degree of hydrolysis and hydrolysis constant of sodium acetate Conductometrically

MAGNETO – CHEMISTRY

14) To determine the magnetic susceptibility and number of unpaired electrons in a given compound.

15) Verification of Weidemann's law using nickel chloride solutions

SURFACE TENSION

16) 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 stalagmomenter

17) Determine the parachor of a solid by stalagmometer

THERMODYNAMICS

18) Determine the partial molar volume of ethanol and water in a given composition by density measurements.

19) To determine heat of neutralization of strong acid and heat of ionization of weak acid calorimetrically.

20) To determine the integral hear of solution of KNO_3

21) To determine the heat of dissociation of benzoic acid in water

22) To determine heat of precipitation of $BaSO_4$

M. Sc. Second Year
Laboratory Course-VII,
Paper– XXVII, CH-503

Marks: 4 Credit **Periods: 132**

CHEMICAL DYNAMICS

1) Investigate the influence of ionic strength on the rate constant of the reaction between $K_2S_2O_8$ and KI (TKC-335)

2) Determine the order of a reaction by I) substitution method (II) fractional change method and (III) differential method

3) Investigate the reaction between bromic acid and hydrochloric acid (TKC 346)

4) Investigate the reaction between H_2O_2 and KI kinetically

5) Investigate the kinetics of iodination of acetone.

PHASE EQUILIBRIA

6) Determine the critical solution temperatur of phenol and water in presence of 1)1`% NaCl 2) 0.5% naphthalene 3) succinic acid

7) Construct the phase diagram of a three- component system containing ethanol benzene and water.

8) Determine the equilibrium constant of the tri- iodide formation in aqueous solution by distribution method.

ADSORPTION

9) Investigate the adsorption of acetic/ oxalic acid by activated charcoal and test the validity of Rreundlich and Langmuir's isotherm

SECTION (A): APPLICATION OF COMPUTER IN CHEMISTRY

10) Calculate the mole fraction of liquid mixture from given data by using Excel– Software

11) Determine the excess molar volume of binary liquid / ternary liquid mixture by using Excel / MATLAB softwere from given data.

12) Calculate mean deviation, relative mean deviation and standard deviiation byusing Excel / MATLAB softwere from given data.

13) Calculate the excess viscosity of binary / ternary liquied mixtures by using Excel /Matlab

14) Plot the graph of Emf Vs volume of titrant added E/V Vs volume of titrant added
from the experimentally observed data by using Excel softwere and justify thenature of graph.

15) Determine proton ligand formation number (nA) dissociation constant (pK) andmetal – ligand stability constant (pL) by using Excel programme.

16) Draw the molecular structure of given molecules using chem. Draw Windows.

17) Draw the graph of ionization potantial Vs. Atomic number or II, III, IV, V, VI row elements and justify the nature.

18) Draw the graph between atomic number Vs I.P. and electro-negativtiy of first group elements by using Excel softwere from given data and justify the nature of the graph.

M. Sc. Second Year
Laboratory Course-VIII,
Paper– XXVIII, CH-504

Marks: 4 Credit **Periods: 132**

PROJECT

The students will develop utilities such as analytical spectra, simulation programmes that will supplement laboratory exercieses in their subject of specialization. For this, variety of small research project designed by the teacher based on the interest of the student and capabilities should be worked out.

SEMINAR

The students will have to give at least one seminar in each semester in their subject of spoecialization. For this submission of synopsis of seminar delivered by every student is compulsory wihcih is to be produced before examiner of practical examination.