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UNIVERSITY OF MUMBAI

Program : M.Sc.

(Choice Based Credit System)

Course : M.Sc. Physical Chemistry

Syllabus for Semester III & IV

(To be implemented from the Academic year 2018-2019)

M.Sc. PHYSICAL CHEMISTRY

SEMESTER III

PSCHP301

Paper I

Chemistry: Polymer, Surface & Photo

UNIT- I: Polymer Chemistry-I **(15L)**

1.1 Introduction: Polymer Science, fundamental terms, historical outline, classification based on: the origin (natural, semi-synthetic, synthetic etc.),the structure (linear, branched, network, hyper branched, dendrimer, ladder, cross linked, IPN),the type of atom in the main chain(homochain,heterochain),the formation(condensation,addition), homo polymers,co polymers(random,alternate,block,graft),the behavior onapplication of heat (thermoplastic and thermosetting),the form and application (plastics, fibre, elastomersandresins). **(05L)**

1.2 Molar Mass: Molecular weight averages, fractionation, molecular weight determination by GPC/SEC,end group analysis, viscometry, vapour phase osmometry, gradientelution, and molecular weight distribution curve**.** **(05L)**

1.3 Types of polymerization: condensation, addition (cationic and anionic)and copolymerization(withkinetics),chain transfer reactions. **(05L)**

Reference Books:

1. *P. Bahadur and N. V. Sastry, Principles of Polymer Science, second edition,NarosaPublishingHouse,2005.*
2. *C. E. Carraher, Jr., Carraher's Polymer Chemistry, 8th edition, CRC Press, New York,2010.*
3. *JoelR.Fried,PolymerScienceandTechnology,Prentice-HallofIndiaPvt.Ltd., 2000.*
4. *V.R.Gowarikar,H.V.ViswanathanandJ.Sreedhar,PolymerScience.NewAge InternationalPvt.Ltd.,NewDelhi,1990.*
5. *F. W. Billmeyer Jr., Text Book of Polymer Science, 3rd edition, John Wiley and Sons,1984.*
6 *V.K.Ahluwalia&A. Mishra, Polymer Science, A text book,Ane-Books Pvt. Ltd,2008.*
7 *R.Sinha, Outline of Polymer Technology manufacture of Polymers, Prenticehall ofIndiaPvt.Ltd.2000*
8 *F.J.Davis,PolymerChemistry,Oxford UniversityPress,2000.*
9 *D.Walton&P.lotimer,Polymer,Oxford UniversityPress,2000.*
10*R.Ypung,IntroductiontoPolymers,Chapman&Hall,reprint,989.*
11*V.Jain.OrganicPolymerChemistry,IVYPublishingHouse,2003.*
12*A.Singh,PolymerChemistry,CampusBookInternational,2003.*

Books for further reading:

1. *J. M. G. Cowie, Polymers: Chemistry and Physics of Modern Materials, 2nd ed. (firstIndianReprint2004),ReplikaPressPvt.Ltd.*
2. *G.S.Misra,IntroductoryPolymerChemistry,NewAgeInternational(P)Limited, Publishers,1993.*
3. *L. H. Sperling, Introduction to Physical Polymer Science. 2nd Edition, John WileyandSons.Inc.*
4. *Hans-GeorgElias,AnIntroductiontopolymerScience,VCH1997.*
5. *Charles E. Seymour, Jr., Seymour/Carraher's Polymer Chemistry, 6th ed., Marcel Dekker, Inc.,2003.*
6. *A. Ravve, Principles of Polymer Science, 2nd ed., Kluwer Academic/Plenum Publishers,NewYork,2000.*
7. *VidyagauriLele, Chemical modification of starch by green process, Techno World Press, 2015.*
8. *VidyagauriLele, Graft copolymers of starch-Synthesis & Characterization, Neeraj Publishing House, 2015.*

UNIT-II Modern Applications of Surface Chemistry (15L)

2.1 Surface active agents and micelle: (08L)

2.1.1 Surface active agents andt their classification,hydrophile-lipophile balance**(02L)**

2.1.2 Micellization: shape and structure of micelles , hydrophobic interaction, critical

Micelles concentration (cmc), factors affecting cmc of surfactants, counter ion binding to micelles,micelle catalysis,reverse micelles. **(04L)**

2.1.3 Emulsions: Solubilization,micro emulsions, characterization of microemulsions, (02L)

Reference Books:

1. M. J. Rosen. Surfactants and Interfacial Phenomena (3rd edn.), John Wiley (2004).

2. Y. Moroi, Micelles: Theoretical and Applied Aspects, (1992) Plenum Press,New York

3.ArunK.Chattopadhyay,KashmiriLalMittal,SurfactantsinSolution,Volume64of Surfactant Science Series,Volume 64 of Lecture Notes in Pure and Applied Mathematics,illustrated,MarcelDekker,1996

4.K.L.Mittal,AmericanChemicalSociety,Micellization,solubilization,and microemulsions,Volume1 Micellization,Solubilization,andMicroemulsions,AmericanChemicalSociety, illustrated,PlenumPress,1977

5.DeepakThassu,MichelDeleers,YashwantPathak,NanoparticleDrugDelivery Systems Volume166ofDrugsandthePharmaceuticalSciencesSeriesillustrated,CRC Press,2007

Reference Books

1. K.R.Lange.Surfactants,HanserPub.(1999).
2. R.Zana(ed.).DynamicsofSurfactantSelf-Assemblies,CRCPress(2005).
3. M.Abe&J.F.Scamehorn.MixedSurfactantSystems,CRCPress(2004).

2.2 Hydrogen storage by Adsorption: (07L)

2.2.1 Hydrogen storage: fundamentals physisorption , temperature and pressure influence,chemisorption,adsorptionenergy,'Electrochemical'adsorption. (03L)

2.2.2. Practical adsorption: storage of hydrogen with carbon materials, activated carbon,graphite graphene,carbon nano structures,fullerene.Carbon nano fibres(CNF) and graphite nano fibers electrochemical storage of hydrogen in carbon materials.(04)

Reference books:

1.Tushar K. Ghosh, Energy Resources and Systems: Volume 2: Renewable Resources,Volume2 of Energy Resources and Systems,Energy Resources and Systems,Springer Link:Bücher,Springer,2011

2.R. Str¨obel a, J. Garche b, P.T. Moseley c, L. J¨orissen b, G. Wolfd. "Review Hydrogen storage by carbon materials." Journal of Power Sources (WWW.Sciencedirect.com) 159 (June 2006): 781–801.

3. Agata Godula-Jopek,Walter Jehle,Joerg Wellnitz,Hydrogen Storage Technologies:New Materials,Transport,and Infrastructure,JohnWiley&Sons, 2012

4. Yury Gogotsi,CarbonNanomaterials,illustratedVolume1of Advanced Materials Series.Advanced Materials and Technologies Series,CRCPress,2006

5.Robert A. Varin,TomaszCzujko,Zbigniew S. Wronski,Nano materials for Solid State Hydrogen Storage FuelCellsandHydrogenEnergyillustratedSpringer,2009

UNIT-III Photo Chemistry-I **(15L)**

3.1 Photo chemical principles: Environmental effect on absorption and emission spectra, properties ofexcited states, excited stateacidity constants, dipole momentsand redox properties, Importance of photochemistry, origin of life, **(04L)**

3.2 Photo physical processes in electronically excited molecules: types of photo physical pathways, types of radiation less transitions, fluorescence emission, fluorescence and structure. Triplet state and phosphorescence emission, delayed fluorescence–etypeandp-typedelayedfluorescence. **(06L)**

3.3 Photo chemical reactions:ketones,olefins conjugated olefins andaromatic compounds, photosynthesis. **(05L)**

Reference Books for Photochemistry

1 C.H.DePuy,O.L.Chapman,Molecular reactions and photo chemistry,Prenticehall of India PVT.LTD.1988.

2 K.K.Rohatgi-Mukherjee. Fundamentals of Photochemistry. Reprint 2002. New Age International Publisher,1978.

UNIT-IV Applications of Fluorescence Phenomena **(15L)**

4.1 Fluorescence sensing: Mechanism of sensing; sensing techniques based on Coalitional quenching, energy transfer, electron transfer; examples of pH sensors glucose sensorsand protein sensors. **(05L)**

4.2 Novel fluorophores: Quantum dots, lanthanides and long-lifetime Metal- ligand complexes. **(05L)**

4.3 Radiative decay engineering: metal enhanced fluorescence**(03L)**

4.4 DNA technology–sequencing. **(02L)**

Reference Books:

1. B. Valeur, Molecular Fluorescence: Principles and Applications, Wiley-VCH (2001).

2. J.R.Lakowicz, Principles of Fluorescence Spectroscopy,Springer(2006).

Reference Book

1. D.L.Andrews &A. A. Demidov, Resonance Energy Transfer, John Wiley & Sons (1999).

Semester – III

PSCHP302

Paper II

Nano chemistry, statistical mechanics &Nuclear chemistry

UNIT-I:Nano chemistry of ,gold,cadmium,selenide. **(15L)**

1.1 Variation of optical and magnetic properties of non material lwith size,shape,surface characteristics and impurities **(04L)**

1.2 Relationship between size and shape of nano materials **(03L)**

1.3 Nano architecture: self assembly and template methods **(03L)**

1.4 Diagnosis and treatment of diseases using nano particles **(03L)**

1.5 Safety and ethics of use of nano particles **(02L)**

UNIT-II Nano chemistry of silica and poly dimethyl siloxane: **(15L)**

2.1 Variation of optical and magnetic properties of nano materials with size, shape, surface characteristics and impurities **(04L)**

2.2 Relationship between size and shape of nano materials. **(03L)**

2.3 Nano architecture:self assembly and template methods. **(04L)**

2.4 Diagnosis and treatment of diseases using nano particles **(04L)**

Reference Books:

1. Ludovico Cademartiri and GeoffreyA.Ozin,Concepts of Nano chemistry,Wiley–VCHVerlagGmbH&co,2009

2.C.Bréchignac,P.Houdy,MarcelLahmani, Nano materials and Nano chemistry, Springer,2007

3.C.N.R.Rao,Achim Müller,Anthony K. Cheetham, Nano materials Chemistry ,John Wiley & Sons, 2007

4.Geoffrey A. Ozin,André C. Arsenault,Ludovico Cademartiri, Nano chemistry: A Chemical Approach to Nano materials, Royal Society of Chemistry (GreatBritain)2, illustrated, Royal Society of Chemistry,2009

Unit- III Statistical Mechanics (15L)

3.1Thermodynamic probability: Combinatral problems, Strilling apporoximation**,** Lagranges method, macro and microstates,ensembles,Boltzmann distribution law.(03)
3.2 Partition functions:Translational,rotational,vibrational,electronic and nuclear partition functions, Expressions for the thermodynamic functions interms of partition function -Internal energy, heat capacity, the Helmholtz and Gibbs functions, Enthalpy, entropy and equilibrium constants. Sackur –Tetrode equation for the entropy of a mono atomic gas. Molecular partition function. **(07L)**

3.3 Maxwell-Boltzmann,Bose-Einstein and Fermi-Dirac statistics. (03L)

3.4 Debye and Einstein theory of specific heats of solids. (02L)

Reference Books:

1. AtkinsP.W,PhysicalChemistry,Oxford UniversityPress,6thedition,1998

2. JohnM.Seddon&JulianD.Gale,Thermodynamics and statistical mechanics, Tutorial Chemistry Textsseries,Vol.10,Royalsociety of Chemistry,2001.

3. Silbey RJ & Alberty RA,Physical Chemistry,3rd edition,John Wiley and sons, Inc.2002.

4. Laidler K.J. and Meiser J.H., Physical Chemistry, 2nd edition, CBS publishers & distributors,1999.

5. B.K.Agarwal and M.Eisner,Statistical Mechanics,(1988)Wiley Eastern,New Delhi.

6. D.A.McQuarrie,Statistical mechanics, (1976)Harper and Row Publishers, New York.

UNIT—IV Nuclear Chemistry (15L)

4.1 Charged particle accelerator- linear accelerator, cyclotron, Betatron, Synchro-cyclotron, synchrotron **(04L)**

4.2 Nuclear forces- characteristics and Meson field theory of nuclear forces **(02L)**

4.3 Nuclear Models-Liquid drop model**,** Fermi Gas Model, Shell Model, Collective Model, Optical Model. **(04L)**

4.4 Applications of Nuclear radiations- geological applications of radioactivity, age of minerals and rocks, age of earth and solar system, medical, industrial and agricultural applications of radiochemistry, positron emission tomography, Radio immune assay. **(05L)**

Reference Books:

1. ***G.Friedlander,J.W.Kennedy.Nuclear and Radio chemistry.Third.John Wiley and sons,,1981.***
2. ***H.J.Arnikar,Essentials of Nuclear Chemistry.second.Wiley Eastern Ltd., 1989.***

SEMESTER-III

PSCHP303

Paper-III

Atomic and Molecular: Structure and Spectroscopy

UNIT-I:Atomic structure **(15L)**

1.1: Introduction to approximate methods in Quantum Mechanics- (09)

1.1.1 Variation Theorem, linear and nonlinear variation functions.

1.1.2 Perturbation Theory, Non degenerate Perturbation Theory, first order wave function correction, first order and second order energy correction.

1.1.3 Application of variation and perturbation theory to ground state of Helium Atom.

1.2:**Multi –electron atoms**:Antisymmetry and Pauli principle, Slater determinants, Hartree. – Fock and configuration interaction wave functions, Slater type orbitals, Gaussian orbitals, orbitals plots, Basis sets. Density functional theory. (06)

UNIT-II Atomic spectroscopy **(15L)**

2.1 Angular momentum, orbital and spin, total angular momentum, total angular momentum (J) of many electron atoms, Russell Saunders (L-S) coupling and J-J coupling, **(04L)**

2.2 Term symbols, term symbols for multi electron atoms like He, Li, Be, B etc. **(04L)**

2.3 Exchange of interactions and multiplicity of states. **(02L)**

2.4 Anomalous Zeeman Effect and Paschen Back effect. **(02L)**

2.5 Atomic spectra and selection rules, energy level diagram of atomic sodium.**(03L)**

UNIT-III: Molecular Structure **(15L)**

3.1 The Born–Oppenheimer approximation **(01L)**

3.2 LCAO method-molecular orbital formation **(01L)**

3.3 Calculation of energy of hydrogen molecule ion using **(05L)**

3.3.1 Valence bond method

3.3.2 Heitler-London treatment

3.3.3 Improvements in Heitler-London treatment

3.4 Electronic structure of polyatomic molecules **(08L)**

3.4.1 Valence bond method for BeH_2, H_2O, NH_3, BH_3 ,CH_4.

3.4.2 Huckel molecular orbital's Theory for–ethylene, Allyl system, cyclopropenyl system and cyclobutadiene. .

Reference Books:

1. ***Laidler and Miser, Physical Chemistry,2nd edition, CBS publishers, New Delhi.(chapters11-14)***
2. ***Silbey and Alberty, Physical Chemistry,3rd edition, JohnWiley and sons, 2000.(Parttwoquantumchemistry)***
3. ***Atkins P.W, Physical Chemistry, Oxford University Press,6th edition,1998.***
4. ***William Kemp, Organic spectroscopy,3rd Edition,ELBS,1996.***
5. ***I.N. Levine, Quantum Chemistry,5th Edition (2000), Pearson Educ. Inc., New Delhi.***
6. ***.D.A.McQuarrie andJ.D.Simon, Physical Chemistry:A Molecular Approach,(1998)Viva Books,NewDelhi.***
7. ***J.N.Murrell,S.F.A.KettleandJ.M.Tedder,ValenceTheory,2(1965),J nd edition ohnViley,NewYork.***
8. ***A.K.Chandra,IntroductoryQuantumChemistry,4McGrawH th edition(1994),Tata ill,NewDelhi***
9. ***D.A.McQuarrie, Quantum Chemistry, Viva Books Private Limited, New Delhi, first Indian ed.,2003.***
10. ***R. K. Prasad, Quantum Chemistry,3rd Ed., New Age International Publishers,2006.***
11. ***James E. House, Fundamentals of Quantum Chemistry, Second Ed.,Academic Press,2005.***
12. ***T.A. Littlefield and N. Thorley,Atomic and Nuclear Physics– An Introduction,Van Nostrand,1979.***

UNIT-IV:Molecular spectroscopy **(15L)**

4.1Rotational spectroscopy: Einstein coefficients, classification of poly atomic Molecules spherical top, symmetric top and asymmetric top molecules, rotational spectra of polyatomic molecules Stark modulated microwave spectrometer. **(03L)**

4.2 Raman Spectroscopy-Classical theory of molecular polarizability, pure rotational, vibrational and vibration-rotation spectra of diatomic and polyatomic molecules polarization and depolarization of Raman lines correlation between IR and Raman spectroscopy instrumentation. **(05L)**

4.3 Electronic Spectra of molecules: Term symbols for linear molecules, selection rules characteristics of electronic transitions-Franck-Condon principle, types of electronic transitions-d-d, vibronic, charge transfer, π-π^*,n-π^*transitions, fate of electronically excited states, fluorescence, phosphorescence, dissociation and pree-dissociation

(07L)

ReferenceBooks

1. **C.N.Banwell and E.M.McCash,Fundamentals of Molecular Spectroscopy,4thEd.,Tata-McGraw-Hill,1994.**
2. **M. L. Gupta, Atomic and Molecular Spectroscopy, New Age International Publishers,2001.**
3. **H.S.Randhawa, Modern Molecular Spectroscopy,McMillanIndiaLtd.,2003**
4. **G.Aruldas, Molecular Structure and Spectroscopy,Prentice-HallofIndia,2001.**

5. J.Michael Hollas, Modern Spectroscopy, 4thEd., John Wiley and Sons,2004.

List of Books for further reading:

1. R.Drago, Physical Methods for Chemists,Saunders, Philadelphia,1992.
2. B.P.Straughan and S.Walker(Eds.),Spectroscopy–Vol1-3,Chapman and Hall,NewYork,1976.
3. R.K.Harris,Nuclear Magnetic Resonance Spectroscopy,Pitman,London,1983.
4. Donald L. Pavia, Gary M. Lampman and George S. Kriz, Introduction to Spectroscopy,3rded., Thomson, Brooks/Cole,2001.
5 John P. Lowe, Quantum Chemistry,3rded.,AcademicPress,NewYork,2006.
6 R. Anantharaman, Fundamentals of Quantum Chemistry, McMillan India Limited, 2001.
7 Mahendra R. Awode, Quantum Chemistry,S. Chandand Co.Ltd.,New Delhi,2002.
8 DavidO. Hayward, Quantum Mechanics for Chemists, Royal Society for Chemistry,2002.
9 Jack Simons, An Introduction to Theoretical Chemistry, Cambridge University Press,2003.
10 Victor M.S.Gil, Orbitals in Chemistry, A Modern Guide to Students, Cambridge University Press, 2000.
11 A.K.Chandra, Introduction to Quantum Chemistry, 4thEd.,Tata-McGraw-Hill, 1994.
12 S.N.Datta Lectures on Chemical Bonding and Quantum Chemistry, Prism Books Pvt.Ltd.,1998.
13 R.McWeeny, Coulson's Valence,3rd.Ed.,Oxford University Press,1979.
14 J.N.Murell,S.F.A.Kettle and J.M.Tedder,The Chemical Bond, Wiley,1985.
15 F.A.Cotton,Chemical Applications of Group Theory,3rdEd., John Wiley and Sons(Asia) Pte. Ltm, 1999.
16 D.C.Harris and M.D.Bertolucci, Symmetry and Spectroscopy, Oxford University.

SEMESTER-III

PSCHPEC-I 304

Advanced Instrumental Techniques

UNIT-I Electron Spectroscopy and Microscopy **(15L)**

1.1 Electron Spectroscopy: principles, instrumentation and applications of the following ESCA (XPS), AUGER, UPS. **(09L)**

1.2 Electron Microscopy: principles, instrumentation and applications of the following: Scanning Probe Microscopes, Scanning Electron Microscope(SEM), Scanning Tunneling electron Microscope(STEM) and Atomic Force Microscope(AFM) **(06L)**

UNIT-II Thermal Methods **(15L)**

2.1Thermogravimetry (TG): Principle and Instrumentation, factors affecting thermo gravimetric curves, Interpretation of thermo gravimetric curves. applications of thermo gravimetry **(04L)**

2.2 Differential thermal analysis(DTA)and Differential scanning calorimetry (DSC): Principle and instrumentation, heat flux and power compensated DSC ,Interpretation of DTA and DSC curves applications of DTA and DSC. **(05L)**

2.3 Enthalpimetric methods **(02L)**

2.4 Thermometric titrations: principle instrumentation and applications **(02L)**

2.5 Evolved gas analysis (EGA): principle and applications. **(02L)**

Reference Books:

1) Skoog DA, West DM, Fundamentals of Analytical Chemistry, Thomson Asia Pvt ltd.,8th Ed,(2004)

Skoog, Holler, Nieman, Principles of Instrumental Analysis, Thomson Asia Pvt ltd.,5th Ed(2003)

1) **Sharma B. K., Instrumental Methods of Chemical Analysis, Goel Publishing House.**
2) **Wendlandt., Thermal Methods, WW John Wiley,(1986).**
3) **Willard Merrit and Settle, Instrumental Methods of Analysis.**
4) **Douglas A.Skoog, Holler & Crouch, Instrumental analysis India edition CENGAGE Learning (EighthIndianReprint2011)**
5) **Robert D.Braun. Introduction to Instrumental Analysis(IndianReprint2006)**
6) **J.W.Dodd, K.Tonge, Thermal Methods. Analytical Chemistry, open Learning.**
7) **Pavia, Lapman, kriz, introduction to Spectroscopy, Thomson Pub.**
8) **H.Straw, & K. walker, Spectroscopy Vol.I&II, Science Paper backs.**
9) **M.Mahindersingh, Analytical chemistry, Instrumental techniques, Dominant Pub. Delhi.**
10) **F.W.Fiefield, & D.Kealey, Principles and Practice of analytical Chemistry, Blackwell Pub.**
11) ***G.W.Ewing,Instrumental methods of Chemical analysis, MacGrawHill.***

UNIT-III Hyphenated Techniques **(15L)**

3.1 Introduction, need for hyphenation, possible hyphenation. **(02L)**

3.2 Interfacing devices and applications of the following: GC-MS,GC-IR,MS-MS,HPLC-

MS, ICP-MS, spectro-electro chemistry and radio-chromatography. **(13L)**

Reference Books:

1 R.P.W.Scott, Tandem Techniques, Wiley India Pvt. Ltd.Reprint2009

2 J.Barker, Analytical chemistry for open learning, Mass spectrometry,WiileyIndiaED.

UNIT-IV Electro-Analytical Methods. (15L)

4.1 Over view of electrode process: Electro-capillary curve and electro-capillary maximum potential. **(02L)**

4.2 Micro electrodes: mercury electrodes: Stationary mercury drop electrode (SMDE).Hanging mercury drop electrode (HMDE), Mercury film electrode (MFE),Carbon paste electrode and chemically modified electrodes. **(03L)**

4.3 Introduction to three electrode system: modern polarography and voltammetry necessity and development of new voltammetric techniques and their comparison with classical DC polarography, **(03L)**

4.4 Voltammetric methods: Sampled DC polarography (TAST), Linear sweep voltammetry (LSV),Cyclic voltammetry (CV), diagnostic criteria of cyclic voltammetry **(07L)**

Reference Books:

1) ***A.J.BardandL.R.Faulkner,Electrochemical Methods,2nd Ed,John Wiley and sons, Asia Pvt. Ltd,(2004)***
2) ***J.J.Lingane , Electro-analytical Chemistry, 2nd Ed, Inter science Publishers, Inc., New York (1958)***
3) ***A.M.Bond, Modern Polarographic Methods in Analytical Chemistry, Marcel Dekker Publishers, Inc., New York,(1980)***
4) ***A.J.Bard(Ed), Electro-analytical Chemistry, Marcel DekkreInc., New York (A series of volumes)..***
5) ***Donald T.Sawyer ,A.Sobkowiak and J.L.Roberts,Jr., Electro chemistry for Chemists, 2nd Ed., John Wiley and Sons, Inc., New York.,(1995).***
6) ***D.A.Skoog, F.J.Holler, J.A.Nieman, Principles of Instrumental analysis, 6th Ed.***
7) ***R.D.Braun.introduction to Instrumental Analysis,MacGrawhill,1987.***
8) ***H.A. Willard, L.L.Merritt, J.A.Dean&F.A.Settle, Instrumnetal methods of analysis, 5th Ed.CBS,1986.***
9) ***M.noel,K.J.Vasu,Cyclic Voltammetry and Frontiers of electro chemistry,IBH, NewDelhi,1990.***

SEMESTER-III

PSCHPEC-II 304

Advanced Instrumental Techniques

UNIT-I Spectral Methods

Principle, instrumentation and applications of the following **(15L)**

1.1 Reflectance spectroscopy **(03L)**

1.2 Photo-acoustic spectroscopy **(03L)**

1.3 Polarimetry : ORD, CD **(04L)**
1.4 Chemiluminescence method **(02L)**
1.5 Nuclear quadruple resonance spectroscopy, ENDOR, ELDOR, EWDOR **(03L)**

UNIT-II Electro-analytical Methods – I
Principles, instrumentation and applications **(15L)**

2.1 Ionselective field effect transistors, bio-catalytic membrane electrodes, disposable multi layer pIon systems, screen–printed electrodes. **(08L)**
2.2 Chrono potentiometry and chrono amperometry **(05L)**
2.3 Fused salt electrolysis **(02L)**

Reference Books:

1) ***A.J.BardandL.R.Faulkner, Electrochemical Methods, 2nd Ed, John Wiley and sons, Asia Pvt. Ltd, (2004).***
2) ***J.J.Lingane, Electro-analytical Chemistry, 2nd Ed, Inter science Publishers, Inc., New York (1958)***
3) ***A.M.Bond,Modern Polarographic Methods in Analytical Chemistry, Marcel Dekker Publishers, Inc.,New York,(1980)***
4) ***A.J.Bard(Ed), Electro-analytica lChemistry, Marcel DekkreInc., NewYork (A series of volumes)..***
5) ***DonaldT. Sawyer ,A.SobkowiakandJ.L.Roberts,Jr.,Electro chemistry for Chemists,2nd Ed.,JohnWileyandSons,Inc.,NewYork.,(1995).***
6) ***D.A.Skoog,F.J.Holler, J.A.Nieman,Principles of Instrumental analysis, 6th Ed.***
7) ***R.D.Braun.introduction to Instrumental Analysis,MacGrawhill,1987.***

8) ***H.A. Willard, L.L.Merritt, J.A.Dean&F.A.Settle, Instrumnetal methods of analysis, 5th Ed.CBS,1986.***
9) ***M.noel,K.J.Vasu,CyclicVoltammetry and Frontiers of electro chemistry,IBH, NewDelhi,1990.***
10) ***P.T.Kissinger,W.R.heinman,LaboratotyTechniques in electro analytical Chemistry,Dekkar,NY.1984.***

UNIT-III Radio-analytical Methods **(15L)**

3.1 Activation analysis-basic principles, fast neutron activation analysis, radio-chemical method inactivation analysis **(04L)**

3.2 Isotopic dilution method-principle and applications**.** **(02L)**
3.3 Auto, x-ray and gamma radiography (**04L)**
3.4 Radiometric Titrations **(03L)**
3.5 Applications of radio-analytical techniques. **(02L)**

References Books for Radioanalytical Methods:

1) ***J.RutickaandJ.Stary, Sub stoichiometry in Radio chemical Analysis, Pergamon Press,(1968)***
2) ***R.A.FairesandG.G.J.Boswell,Radio isotope Laboratory Technique,4th, Ed, Rutterworths; London, (1981)***
3) ***D.Brune, B. Forkman, B.Person, Nuclear Analytical Chemistry, Chartwell- Bratt Ltd.,(1984)***
4) ***Maheshwar Sharon and Madhuri Sharon, NuclearChemistry, Ane Books Pvt. Ltd.(2009)***
5) ***Nuclear Chemistry By Arnikar***

UNIT-IV Pulse polarography: **(15L)**

4.1 Normal pulse polarography(NPP), Differential pulse polarography(DPP), Double differential pulse polarography(DDPP), **(08L)**
4.2 Sinusoidal AC polarography, Square wave polarography (**05L)**
4.3 Applications of electrochemical methods in Organic synthesis**.** **(02L)**

References :

1) ***M. Noel and KI.Vasu, Cyclic Voltammetry and the frontiers of Electrochemistry, IBH, NewDelhi,(1990)***
2) ***A.M.Bond, Modern Polarographic Methods in Analytical Chemistry, Marcel Dekker Publishers, Inc., New York,1980.***
3) ***A. J. Bard and Faulkner, Electrochemical Methods, 2nd Ed, John Wileyand Sons (Asia) Pvt. Ltd., 2004.***

Practicals

SEMESTER-III

PSCHP3P1

1. To determine of the formula of the copper (II) ammonia complex by partition method.

2 .To determine the transport no. of copper(II)ions by Hittorf's method.

3. To determine the isoelectric point of gelatin by viscosity measurement.

PSCHP3P2

1. To determine the mean ionic activity coefficient of zinc chloride by emf method.

2.To construct the phase diagram for a two component system forming a simple eutectic..

Non instrumental

3. To determine the equilibrium constant for the reaction

$$CaSO_4\,(s) + 2Ag^{+1}\,(aq) = Ag_2SO_4(s) + Ca^{-2}\,(aq)$$

4.To determine the partial molar volume of ethanol.

PSCHP3P3

1. Determination of the energy of activation and other thermodynamic parameters of activation for the acid catalyzed hydrolysis of methyl acetate.

2.To determine the proton ligand stability constant of an organic acid and metal ligand stability constant of its complex by pH measurement.

Conductometry

1 To determine the molar conductance of a weak electrolyte at infinite dilution hence to determine its dissociation constant.

2To titrate potassium ferrocyanide with zinc sulphate and hence to determine the formula of the complex.

Potentiometry

1To determine the E^0 of the quinhydrone electrode.

2 To determine the formula of the zinc(II)ferrocyanide complex by titration of Zn(II) sulphate with potassiumferrocyanide.

p H metry

1To estimate the amount of hydrochloric acid and acetic acid in a mixture by titration with an alkali using a pH meter.

2To determine hydrolysis constant and degree of hydrolysis of ammonium chloride and hence to estimate the dissociation constant of the base.

PSCHP3P4

1. To determine the molar mass of a nonvolatile solute by cryoscopic method.

Colorimetr & spectrophotometry

1.To determine the ionization constant of bromophenol blue

2. Tostudycomplexformationbetweennickel(II)witho-phenanthroline.

3. To determine the rate constant and the order of the reaction between persulphate and iodide ions.

1.The candidate is expected to submit a journal certified by the Head of the Department/institutionatthetimeofthepracticalexamination.

2.A candidate will not be allowed to appear for the practical examination unless he / she produces a certified journal or a certificate from the Head of the institution/department stating that the journal is lost and the candidate has performed the required number of experiments satisfactorily. The list of the experiments performed by the candidate should be attached with such certificate.

3.Use of non-programmable calculator is allowed both at the theory and the practicalexamination.

List of reference Books for Practicals:

1. ***B.VishwanathanandP.S.Raghavan,PracticalPhysicalChemistry,Viva BooksPrivateLimited,2005.***
2. ***A.M.JamesandF.E.Prichard,PracticalPhysicalChemistry,3rded., Longman,1974.***
3. ***B.P.Lewitt(ed.),Findlay'sPracticalPhysicalChemistry,9thed.,1973.***
4. ***C.D.BrennanandC.F.H.Tipper,ALaboratoryManualofExperimentsin PhysicalChemistry,McGraw-Hill,1967.***
5. ***F.Daniel&Others,ExperimentalPhysicalchemistry,19665,KogakashaCoLtd.,Tokyo.***

SEMESTER -IV

PSCHP401

Paper-I

Chemistry: Polymer, Green, Biophysical and Applied.

Unit I: Polymer Chemistry-II (15L)

1.1 Polymers in solid state – Transitions (glass transition and crystalline melting temperature), crystalline behaviour, factors affecting crystallinity, polymer blends and Alloys. **(03L)**

1.2 Identificationandcharacterizationofpolymers:Chemical analysis- End group analysis; Physical analysis by Spectral methods: IR, UV, Ramam, NMR, X-ray diffractionanalysis,Microscopic methods: SEM, TEM, Thermal analysis-TGA,DTA, DSC. **(06L)**

1.3 Properties of polymers: Thermal (glass transition temperature, and its determination),mechanical(deformationandfracture)effectsinpolymers,viscoelasticity surface (surface tension, hardness, friction, abrasion), physical (Impactstrength,Tensilestrength,solubility) of polymers, weatherability, rheology and mechanical models, mechanical behavior, Rubber elasticity, **(04L)**

1.4 Polymer degradation and stabilization: Oxidative, thermal, radiation, Biodegradation **(02L)**

Unit II: Polymer Chemistry-III (15L)

2.1Techniquesofpolymerization:Bulkpolymerization,solutionpolymerization,suspensionpolymerization,emulsionpolymerizations, **(03L)**

2.2Thermodynamicsofpolymersolutions:Solubility parameter, thermodynamics of mixing**,theta temprature (02L)**

2.3 Polymer technology: **(05L)**

2.3.1 Polymer auxiliaries, plasticizers, heat Stabilizers, colorants, flame retardants. F**illers, reinforcements.**

2.3.2 Elastomers: Introduction, Processing, Rubber Types, Vulcanization, Properties.Reclaiming.

2.3.3 Fibers: Introduction, production, Fiber spinning, Textile fibers, Industrial fibers, recycling.

2.3.4 Films sheets: Introduction and processing techniques (injection and blow moulding extrusion),Recyling of plastics.

2.4 Properties and applications of some commercially important polymers. Carbon chain polymers- Polyolefins, ABS group, elastomers, vinyl polymers, acrylic polymers, heterochain polymers- polyethers, polycarbonates, polysaccharides, polyamides fluoropolymers, Resins (epoxy, alkyd, phenol-formaldehyde and urea-formaldehyde), Silicones, polyphosphazenes, sulphur containing polymers **(05L)**

Reference Books:

1. P. Bahadur and N. V. Sastry, Principles of Polymer Science, second

edition,NarosaPublishingHouse,2005.

2. *C. E. Carraher, Jr., Carraher's Polymer Chemistry, 8th edition, CRC Press, New York,2010.*
3. *JoelR.Fried,Polymer Science and Technology, Prentice-Hall of India Pvt. Ltd., 2000.*
4. *V.R.Gowarikar, H.V.Viswanathan and J.Sreedhar,Polymer Science.New Age International Pvt.Ltd., New Delhi,1990.*
5. *F. W. Billmeyer Jr., Text Book of Polymer Science, 3rd edition, John Wiley and Sons,1984.*
6. *V.K.Ahluwalia&A. Mishra, Polymer Science, A text book,Ane Books Pvt. Ltd,2008.*
7. *R.Sinha, Outline of Polymer Technology manufacture of Polymers, Prenticehall ofIndiaPvt.Ltd.2000*
8. *F.J.Davis,Polymer Chemistry, Oxford university Press,2000.*
9. *D.Walton&P.lotimer,Polymer, Oxford university Press,2000.*
10. *R.Ypung,Introduction to Polymers,Chapman&Hall,reprint,1989.*
11. *V.Jain.OrganicPolymerChemistry, IVY Publishing House,2003.*
12. *A.Singh,Polymer Chemistry,Campus BookInternational,2003.*
13. ***Books for further reading:***

1. *J. M. G. Cowie, Polymers: Chemistry and Physics of Modern Materials, 2nd ed. (firstIndianReprint2004),Replika Press Pvt. Ltd.*
2. *G.S.Misra, Introductory Polymer Chemistry, New Age International (P) Limited, Publishers,1993.*
3. *L. H. Sperling, Introduction to Physical Polymer Science. 2nd Edition, John Wiley and Sons.Inc.*
4. *Hans-Georg Elias,An Introduction to polymer Science, VCH 1997.*
5. *Charles E. Seymour, Jr., Seymour/Carraher's Polymer Chemistry, 6th ed., Marcel Dekker, Inc.,2003.*
6. *A. Ravve, Principles of Polymer*

UNIT-IIIBio-physical Chemistry and Green Chemistry (15L)

3.1 Biophysical Chemistry (08)

3.1.1 Introduction to Complex Biomolecules: Proteins, enzymes, DNA, RNA, polysaccharides andlipids.chirality and pH dependence of biomolecules. **02L)**

3.1.2 Biosensors : Enzyme based, Electrochemical, immunosensor, fluorescence, optical, Piezoelectric Biosensors **(02L**)

3.1.3 Electrophoresis (Technique for bio-molecular study) : Principle and factors affecting electro-phoreticmobility, zone electrophoresis–Paper electrophoresis,cellules acetate electrophoresis, Gel electrophoresis. capillary Electrophoresis, Application of electrophoresis. **(04L)**

Reference Books:

1. U.N Dash,.AText Book of Biophysical Chemistry,Macmillan India Ltd

2. Gurtu and Gurtu, Biophysical Chemistry, Pragati Prakashan.

3. R.P.Budhiraja,Separation chemistry,New Age International(P)Limited,Publisher

4. Avinash Upadhyay, Kakoti Upadhyay, Nirmalendu Nath.Biophysical Chemistry Principles and Techniques Himalaya

5.Susan R.Mikkelson ,Eduardo Corton, Bioanalytical Chemistry, Wiley Interscience.08Science,2nd ed.,Kluwer Academic/Plenum Publishers, New York,2000.

3.2 Green Chemistry: (07L)

3.2.1 Recapitulation of principles of green chemistry, Waste minimization techniques. (01L)

3.2.2 Catalysis and Green Chemistry: Phase transfer catalysts, biocatalyst, photo catalysis. 02L)

3.2.3 Organic solvents, solvent free system, supercritical fluid, ionic liquid, their characteristics,use as catalyst and solvents. 02L)

3.2.4 Alternative energy sources for initiation and execution of chemical reaction: Microwave and sonochemistry. 02L)

Reference Books:

1. MikeLancaster, Green Chemistry An Introductory Text, Royal Society of Chemistry.

2. V.K.Ahluwalia, M.Kidwai, Kluwer Academic Publisher.

UNIT-IV Photochemistry-II: Kinetics and Applications (15L)

4.1: Photophysical Kinetics of bimolecular processes. (10L)

4.1.1: Mechanism of fluorescence quenching.

4.1.2:Collisions in solutions

4.1.3: Kinetics of collisional quenching and Stern-Volmer equation and deviations from Stern Volmer equation,

4.1.4: Concentration dependence of quenching and excimer formation

4.1.5: Quenching by added substances–charge transfer mechanism and energy transfe rmechanism.

4.2: Solar Cells: photovoltaic and photogalvanic cells; photoelectron chemistry; prospects of solar energy conversion and storage,organic solar cells. **05L)**

Reference Book:

K.K.Rohatgi-Mukherjee. Fundamentals of Photochemistry.Reprint 2002. New AgeInternationalPublisher,1978.-

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Semester-IV

PSCHP402

Paper-II
Material Science, network and irreversible thermodynamics,

UNIT-I Metals and alloys: **(15L)**

1.1 Solidification of metals and alloys-homogeneous and heterogeneous nucleation Growth of crystals, growth of silicon single crystal. **(04L)**

1.2 Metallic solid solutions-substitutional and interstitial solid solutions. **(03L)**

1.3 Crystalline imperfections-point ,line and boundary defects **(04L)**

1.4 Atomic diffusions in solids-diffusion mechanisms, steady state and non-steady state diffusions,-impurity diffusion into silicon wafers for integrated circuits.(**04L)**

UNIT-II Mechanical properties of solid materials **(15L)**

2.1 Stress and strain in metals- Engineering stress and engineering strain, shear stress and shear strain, the tensile test and engineering stress -strain diagram, modulus of elasticity, yield strength. **(05L)**

2.2 Hardness and hardness testing plastic deformations of metals in single crystals plastic deformation of polycrystalline metals, solid solution strengthening of metals.

2.3 Fracture of metals-ductile and brittle fracture ,toughness and impact testing, fatigue of metals, the creep test ,creep-rupture test. **(05L)**

Reference Books :

1. ***WilliamF.Smith, Principles of Material Science and Engineering, 3rd edition, McGraw–HillInc.1996.***
2. ***Keer H.V, Principles of the Solid State, first reprint, Wiley Eastern Limited, 1994.***
3. ***Principles of Material science and engineering, 3rd edition, McGraw–Hill Inc.1996.***

List of Books for further reading:

1. ***A.R.West,Solid State Chemistry and its Applications,John Wiley and Sons (Asia) Pvt.Ltd.,***
2. ***L.E.Smart and E.A.Moore, Solid State Chemistry–An Introduction,3rdEd., Taylor and Francis, 2005.***
3. ***V.Raghavan,Materials Science and Engineering, Fifth Ed.,Prentice-Hall of India Pvt. Ltd.,NewDelhi,2004.***
4. ***WilliamD.Callister,Jr.,Materials Science and Engineering, An Introduction, Fifth Ed.,John Wiley and Sons (Asia)Pvt.Ltd.,2001.***
5. ***S.O.Pillai, Solid State Physics, Fifth Ed., New Age International Publishers, 2002.***
6. ***Leonid V.Azaroff, Introduction to Solids, Tata-McGraw-Hill Publishing Co.Ltd., New Delhi, 1977.***
7. ***Sandra E.Dann, Reactions and Characterization of Solids, Royal Society of Chemistry, 2000.***
8. ***C.N.R.RaoandJ.Gopalakrishnan, New Directions in Solid State Chemistry, Seconded.,Cambridge University Press,1997.***
9. ***N.B.Hannay,Solid State Chemistry,Prentice Hall of India, New Delhi,1976.***
10. ***M.AliOmer, Elementary Solid State Physics,5thIndian Reprint, Pearson Education, Inc., 1999.***

Unit III Lasers and super conductors **(15L)**

3.1 Lasers in chemistry **(10L)**

3.1.1 General principles of LASER action-Population Inversion, cavity and mode characteristics, Q-switching, Modelocking. **(02L)**

3.1.2 Practical lasers- Solid state lasers-Ruby, neodymium, gas lasers-He-Ne, Ar, Kr, Carbon dioxide, Chemical and exciplex Lasers,Dye lasers LED and Semiconductor Lasers**.** **05L)**

3.1.3 Applications of Lasers in chemistry: Spectroscopy at high photon fluxes, collimated beams, Precision specified transitions, Isotope separation, Study of fast reactions using pulsed techniques**.** **(03L)**

Reference Book:

.Atkins P.W, Physical Chemistry, Oxford University Press, 6th edition, 1998.

3.2 Super conducting solid materials **(05L)**

Band theory of electrical conductivity, Bardeen-Cooper-Schriffer Theory of super conductivity,the superconducting state, High critical temperature super conductors, magnetic properties of superconductors.

Unit IV **(15L)**

4.1 Non-equilibrium thermodynamics：

4.1.1 Features of non-equilibrium thermodynamics, second law of thermodynamics, uncompensated heat and its relation to thermodynamics function. **(02L)**

4.1.2 Entropy production and its rate. Entropy production in heat transfer process and during mixing of gases.Entropy production and efficiency of galvanic cell.**(04L)**

4.1.3 Onsagers theory: Reciprocal relation, principle of microscopic reversibility. Coupled and uncoupled reactions and their condition.**(05L)**

4.1.4 Transport phenomena across membranes. Electro kinetic effect and thermo mechanical effects.**(04L)**

Reference Books:

1. ***D.A.McQuarrieand J.D.Simon, Molecular Thermodynamics, Viva Books Private Limited, First Indian Ed.,2004.***
2. ***D.A.McQuarrieand J.D.Simon,Physical Chemistry,A Molecular Approach, Viva Books Private Limited, First South Asian Ed.,1998.Chap.***
3. ***E.D.Kaufmann, Advanced Concepts in Physical Chemistry, McGraw-Hill,1966.***
4. ***Robert P.H.Gasser and W.Graham Richards, An Introduction to Statistical Thermodynamics,World Scientific Publishing Co.Pte.Ltd.,1995.***
5. ***C.Kalidas and M.V.Sangaranarayan, Non-Equilibrium Thermodynamics, Principles and Applications, McMillanIndia Ltd.,2002.***

List of Books for further reading:

1. ***M.Dole, An Introduction to Statistical Thermodynamics, Dover, NewYork,1986.***

2. ***W. Kauzmann, Thermodynamics and Statistics: with applications to gases,W. A. Benjamin,NewYork,1967.***
3. ***M. C. Gupta, Statistical Thermodynamics, 2nd. Ed., New Age International Publishers, New Delhi,1998.***
4. ***S. Glasstone, Theoretical Chemistry, Affiliated East–West Press Pvt. Ltd., New Delhi, 1973.***
5. ***S. Glasstone, Thermodynamics for Chemists, Affiliated East–West Press Pvt. Ltd.,New Delhi,1964.***
6. ***R. Hasse, Thermodynamics of Irreversible Processes, Addison Wesley London,1969.***
7. ***I.Prigogine, Introduction to Thermodynamics of Irreversible Processes,3rded., Interscience ,NewYork, 1967.***

PRACTICALS

SEMESTER-IV

PSCHP403

Paper-III

Symmetry &Spectroscopy

UNIT-I: Symmetry in Chemistry **(15L)**

1.1 Recapitulation: point groups, character tables **(02L)**

1.2 Reduction formula, application of reduction formula to vibrational modes of water molecule**.** **(02L)**

1.3 Application in vibrational spectroscopy, selection rules for IR spectroscopy for molecules such as H_2O, CO_2, HF, H_2 **(03L)**

1.4 Application to Raman spectra, selection rules, comparison of IR and Raman selection rules, general approach to vibrational spectroscopy. **(02L)**

1.5 Symmetry in chemical bonding: symmetry adapted linear combination of _molecular orbitals, H_2^+,H_2, LiH, BeH_2, BH_3, CH_4, molecular orbital energy, and bond order. **06L)**

Reference Books :

1 ***K.Veera Reddy, Symmetry and Spectroscopy of molecules,2nded,new age International publishers.***
2 ***U.C.Agarwala,H/L/Nigam,S.Agarwal, S.S.Kalra, Molecular symmetry in Chemistry via group theory, 2013, Ane Books Pvt.ltd.***
3 ***H.N.Dass,symmetry and group theory for chemists,2004 Asian Books Pvt.Ltd.***
4 ***K.V.Raman, group theory and its applications to Chemistry,1980,Tata MacGrawhillPub.Co.Pvt.Ltd.***
5 ***P.K.Bhattacharya, Group theoryand its chemical applications,1999,Himalaya, Pub.House.***
6 ***F.A.Cotton, Chemical applications ofGroup Theory, Wiley Student Ed., 2006, JohnWiley and Sons,(Asia) Pvt.Ltd.***
7 ***R.L.Carter, Molecular symmetry and Group theory, Wiley Student Ed.,1996,John Wiley and Sons, (Asia) Pvt.Ltd.***
8 ***S.Swarnalakshmi, T.saroja, R.M.Ezhilarisi, A simple approach to Group theory in chemistry, 2008, Universities Press (India) Pvt. Ltd.***

UNIT-II N.M.R.Spectroscopy-I **(15L)**

2.1 A review of one dimensional NMR spectroscopy. **(01L)**

2.2 Spin-relaxation.Nuclear Overhauser Effect (NOE).polarization transfer. **(03L)**

2.3 Two-dimensional NMR.Correlated spectroscopy(COSY) **(03L)**

2.4 NuclearOverhauser effect Spectroscopy(NOESY) **(02L)**

2.5 Hetero nuclear correlation Spectroscopy(HETCOR) **(02L)**

2.6 Solid-stateNMR **(02L)**

2.7 Magnetic Resonance Imaging(MRI) **(02L)**

UNIT-III ESR and Mossbauer Spectroscopy **(15L)**

3.1Electron spin Resonance Spectroscopy- **(10L)**

3.1.1 Basic principle, hyperfine splitting(isotropicsystems); (02)

3.2.2 G-value and the factors affecting thereof; interactions affecting electron energies in paramagnetic complexes (Zero-field splitting and Kramer's degeneracy); (03L)

3.3.3 An isotropic effects (the g-value and the hyperfine couplings);The EPR of triplet states; Structural applications to transition metal complexes. (02L)

3.4.4 Fundamentals and hyper fine splitting, application to study of free radicals spin densities McConnell relationship Zero field splitting. (03L)

3.2 Mossbauer Spectroscopy: **(05L)**

Principles, Recoille emission and absorption of γ-rays, experimental methods, isomer shift, hyperfine structure (quadrupole interaction), magnetic hyperfine interaction, applications.

Reference Books:

1. ***C.N.Banwell and E.M.McCash, Fundamentals of Molecular Spectroscopy, 4th Ed., Tata-McGraw-Hill,1994.***
2. ***M. L. Gupta, Atomic and Molecular Spectroscopy, New Age International Publishers,2001.***
3. ***H.S.Randhawa, Modern Molecular Spectroscopy, McMillan India Ltd.,2003***
4. ***G.Aruldas, Molecular Structure and Spectroscopy, Prentice-HallofIndia,2001.***
5. ***J.MichaelHollas, Modern Spectroscopy ,4thEd.,John Wiley and Sons,2004.***

List of Books for further reading:

1. ***R.Drago,Physical Methods for Chemists, Saunders ,Philadelphia,1992.***
2. ***B. P. Straughan and S. Walker (Eds.), Spectroscopy – Vol 1-3, Chapman and Hall, New York,1976.***
3. ***R. K. Harris, Nuclear Magnetic Resonance Spectroscopy, Pitman, London, 1983.***
4. ***Donald L. Pavia, Gary M. Lampman and George S. Kriz, Introduction to Spectroscopy,3rd ed.,Thomson,Brooks/Cole,2001.***

UNIT-IV ^{13}C-N.M.R.Spectroscopy **(15L)**

4.1 Elementary ideas, instrumental difficulties, FT technique advantages and disadvantages. proton noise decoupling technique advantages and disadvantages, off-resonance technique. **(05L)**

4.2 Chemical shifts of solvents, factors affecting chemical shifts, analogy with ^{1}HNMR.

(03L)

4.3 Calculations of chemical shift of hydrocarbons, effect of substituent's on chemical shifts, different types of carbons (alkene, alkyne and allene). **(03L)**

4.4 Chemical shift of aromatic carbons and effect of substituent. **(02L)**

4.5 Chemical shifts of carbonyl, nitrile, and oxime carbons. **(02L)**

Reference Books:

1. ***A.E. Derome, Modern NMR Techniques for Chemistry Research, Pergamon,Oxford(1987)***
2. ***J.K.M. Sanders and B.K. Hunter, Modern NMR Spectroscopy, 2nd edition (1993), Oxford University Press, Oxford.***
3. ***R.K.Harris,Nuclear Magnetic Resonance Spectroscopy,(1986) Addison-Wesley, Longman Ltd.,London***
4. ***Organic spectroscopy by William Kemp,3rdEdition, ELBS, 1996.***

Course Code: PSCHPOC-I 404
Paper – IV (INTELLECTUAL PROPERTY RIGHTS & CHEMINFORMATICS)

Unit 1: **[15L]**

Introduction to Intellectual Property: [2L]

Historical Perspective, Different types of IP, Importance of protecting IP.

Patents: [5L]

Historical Perspective, Basic and associated right, WIPO, PCT system, Traditional Knowledge, Patents and Health care-balancing promoting innovation with public health, Software patents and their importance for India.

Industrial Designs: [2L]

Definition, How to obtain, features, International design registration.

Copyrights: [2L]

Introduction, How to obtain, Differences from Patents.

Trade Marks: [2L]

Introduction, How to obtain, Different types of marks – Collective marks, certification marks, service marks, trade names etc.

Geographical Indications: [2L]

Definition, rules for registration, prevention of illegal exploitation, importance to India.

Unit 2: [15L]

Trade Secrets: [2L]

Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection.

IP Infringement issue and enforcement: [2L]

Role of Judiciary, Role of law enforcement agencies – Police, Customs etc.

Economic Value of Intellectual Property: [2L]

Intangible assests and their valuation, Intellectual Property in the Indian context – Various Laws in India Licensing and Technology transfer.

Different International agreements:

(a) World Trade Organization (WTO): [5L]

(i) General Agreement on Tariffs and Trade (GATT), Trade Related Intellectual Property Rights (TRIPS) agreement

(ii) General Agreement on Trade Related Services (GATS) Madrid Protocol.

(iii) Berne Convention

(iv) Budapest Treaty

(b) Paris Convention [6L]

WIPO and **TRIPS, IPR** and Plant Breeders Rights, IPR and Biodiversity.

Unit III: [15L]

Introduction to Cheminformatics: [5L]

History and evolution of cheminformatics, Use of Cheminformatics, Prospects of cheminformatics, Molecular modeling and structure elucidation.

Representation of molecules and chemical reactions: [5L]

Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification.

Searching Chemical Structures: [5L]

Full structure search, sub-structure search, basic ideas, similarity search, three dimensional search methods, basics of computation of physical and chemical data and structure descriptors, data visualization.

[15L]

Unit IV:

Applications:

Prediction of Properties of Compound, Linear Free Energy Relations, Quantitative Structure – Property Relations, Descriptor Analysis, Model Building, Modeling Toxicity, Structure – Spectra correlations, Prediction NMR, IR and Mass spectra, Computer Assisted Structure elucidations, Computer assisted Synthesis Design, Introduction to drug design, Target Identification and Validation, Lead Finding and Optimization, analysis of HTS data, Virtual Screening, Design of Combinatorial Libraries, Ligand-based and Structure based Drug design, Application of Cheminformatics in Drug Design.

REFERENCES:

1. Andrew R. Leach & Valerie J. Gillet (2007) *An Introduction to Cheminformatics.* Springer: The Netherlands.
2. Gasteiger, J. & Engel, T. (2003) *Cheminformatics: A textbook*. Wiley–VCH
3. Gupta, S. P. *QSAR and Molecular Modeling.* Springer-Anamaya Pub.: New Delhi.

Course Code: PSCHPOC-II 404

PAPER – IV: RESEARCH METHODOLOGY

Unit 1:

Print:

Primary, Secondary and Tertiary sources.

Journals:

Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text-books, current contents, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples.

Digital:

Web sources, E-journals, Journal access, TOC alerts, Hot articles, Citation Index, Impact factor, H-index, E-consortium, UGC infonet, E-books, Internet discussion groups and communities, Blogs, preprint servers, Search engines, Scirus, Google Scholar, ChemIndustry, Wiki-databases, ChemSpider, Science Direct, SciFinder, Scopus.

Information Technology and Library Resources:

The Internet and World wide web, Internet resources for Chemistry, finding and citing published information.

Unit II: DATA ANALYSIS

The Investigative Approach:

Making and recording Measurements, SI units and their use, Scientific methods and design of experiments.

Analysis and Presentation of Data:

Descriptive statistics, choosing and using statistical tests, Chemometrics, Analysis of Variance (ANOVA), Correlation and regression, curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, general polynomial fitting, linearizing transformations, exponential function fit, r and its abuse, basic aspects of multiple linear regression analysis.

Unit III: METHODS OF SCIENTIFIC RESEARCH AND WRITING SCIENTIFIC PAPERS

Reporting practical and project work, Writing literature surveys and reviews, organizing a poster display, giving an oral presentation.

Writing Scientific Papers:

Justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work, writing ethics, avoiding plagiarism.

Unit IV: CHEMICAL SAFETY & ETHICAL HANDLING OF CHEMICALS

Safe working procedure and protective environment, protective apparel, emergency procedure, first aid, laboratory ventilation, safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmospheric pressur, safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives, identification, verification and segregation of laboratory waste, disposal of chemicals in the sanitary sewer system, incineration and transportation of hazardous chemicals.

REFERENCES:

1. Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J., & Jones, A., (2011), *Practical skills in Chemistry*, 2nd Ed., Prentice Hall, Harlow.
2. Hibbert, D. B. & Gooding, J. J. (2006) *Data Analysis for Chemistry* Oxford University Press.
3. Topping, J., (1984) *Errors of Observation and their Treatment* 4th Ed., Chapman Hill, London.
4. Harris, D. C. (2007) *Quantative Chemical Analysis* 6th Ed., Freeman Chapters

3-5
5. Levie, R. De. (2001) *How to use Excel in Analytical Chemistryand in general scientific data analysis* Cambridge Universty Press.
6. Chemical Safety matters – IUPAC-IPCS, (1992) Cambridge University Press.
7. OSU Safety manual 1.01

Semester –IV

PSCHP4P1

1.To determine the formula of the zinc(II) ammonia complex by partition

method.

2 Determination of the transport no. of silver(I) ions by Hittorf's method.

.**Conductometry**.

1.To determine the composition of a mixture of hydrochloric acid, potassium chloride and ammonium chloride by titration with sodium hydroxide and silver nitrate.

2.To determine ΔG, $\Delta H$and ΔS of dissolution of a sparingly soluble salt by conductometry.

pHmetry

1 To determine K_1 and K_2 of a dibasic acid by titration with a base.

2 To determine dissociation constant of p-nitro phenol.

PSCHP4P2

1. To construct the phase diagram for a two component system forming a compound

2. To determine the energy of activation and other thermodynamic parameters of activation for the reaction between persulphate and potassium iodide.

3. To determine the effect of ionic strength of a solution on the reaction between potassium persulphate and potassium iodide.

4. To study the order of the reaction between bromate and bromide.

5. To determine the van't Hoff's factor by cryoscopic method.

Potentiometry

1. To determine the liquid junction potential with a concentration cell with and without transference.

PSCHP4P3

Interpretation of spectra/data:

1. Interpretation of vibrational-rotational spectra of rigid and non-rigid diatomic molecules

2. Interpretation of electronic spectra of diatomic molecules.
3. Interpretation of electronic spectra ofsimple polyatomic molecules.
4. Interpretation of NMR,ESR spectra.
5. Interpretation of Mössbauer spectra.
6. Analysisof XRD pattern of cubic system
7. Interpretation of DTA, TG, and DTG curves

PSCHP4P4

Project Evaluation

List of reference Books for Practicals:

a. ***B.VishwanathanandP.S.Raghavan,PracticalPhysicalChemistry,Viva BooksPrivateLimited,2005.***
b. ***A.M.JamesandF.E.Prichard,PracticalPhysicalChemistry,3rded., Longman,1974.***
c. ***B.P.Lewitt(ed.),Findlay'sPracticalPhysicalChemistry,9thed.,1973.***
d. ***C.D.BrennanandC.F.H.Tipper,ALaboratoryManualofExperimentsin PhysicalChemistry,McGraw-Hill,1967.***
e. ***F.Daniel&Others,ExperimentalPhysicalchemistry,19665,Kogakasha CoLtd.,Tokyo.***

Note:

1. The candidate is expected to submit a journal certified by the Head of the Department/institutionatthetimeofthepracticalexamination.

2. A candidate will not be allowed to appear for the practical examination unless he / she produces a certified journal or a certificate from the Head of the institution/department stating that the journal is lost and the candidate has performed the required number of experiments satisfactorily. The list of the experiments performed by the candidate should be attached with such certificate.

3. Use of non-programmable calculator is allowed both at the theory and the practicalexamination.