AC 27/2/13

Item no. 4.122

UNIVERSITY OF MUMBAI

Syllabus for Semester III and IV
Program: M.Sc.(PSCHP)
Course: Physical Chemistry

Credit based semester and grading system with
effect from the academic year 2013-2014

UNIVERSITY OF MUMBAI

Draft Syllabus

M.Sc. PHYSICAL CHEMISTRY Semester III and IV
Credit Based Semester and Grading System
To be implemented from the Academic year 2013-2014

SEMESTER III

Course Code	UNIT	TOPICS	Credits	L/Week
PSCHP301	I	Polymer chemistry-I	4	1
	II	Modern Applications of Surface Chemistry		1
	III	Photochemistry		1
	IV	Applications of Fluorescence phenomena		1
PSCHP302	I	Spectral Methods-I	4	1
	II	Thermal Methods		1
	III	Radio-analytical methods		1
	IV	Electro-analytical methods		1
PSCHP303	I	Nanochemistry of gold and cadmium selenide	4	1
	II	Nanochemistry of silica and polydimethylsiloxane		1
	III	Statistical Mechanics		1
	IV	Nuclear chemistry		1
PSCHP304	I	Atomic structure	4	1
	II	Atomic Spectroscopy		1
	III	Molecular structure		1
	IV	Molecular Spectroscopy		1
PSCHP3PI PSCHP3P2 PSCHP3P3 PSCHP3P4	Practicals		8	16

SEMESTER IV

Course Code	UNIT	TOPICS	Credits	L / Week
PSCHP401	I	Polymer chemistry-II	4	1
	II	Biophysical chemistry		1
	III	Polymer & Green chemistry		1
	IV	Photochemistry : Kinetics &Applications		1
PSCHP402	I	Spectral Methods-II	4	1
	II	Electro-analytical methods-II		1
	III	Hyphenated Techniques		1
	IV	Electro-analytical Methods-III		1
PSCHP403	I	Metals and alloys		1
	II	Mechanical properties of solid materials		1
	III	Lasers &Superconductors		1
	IV	Network &Non equilibrium thermodynamics		1
PSCHP404	I	Symmetry in Chemistry		1
	II	N.M.R. Spectroscopy-		1
	III	Spectroscopy		1
	IV	^{13}C N.M.R. Spectroscopy		1
PSCHA4P1 PSCHA4P2 PSCHA4P3 PSCHA4P4	practicals		8	16

1. The candidate is expected to submit a journal certified by the Head of the Department / institution at the time of the practical examination.
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 practical examination.

UNIVERSITY OF MUMBAI
M.Sc
Physical Chemistry
(From the academic year 2013-14)

Semester III

PSCHP-301

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, hetercohain),the formation (condensation, addition), homopolymers, copolymers (random, alternate, block, graft),the behaviour on application of heat (thermoplastic and thermosetting),the form and application (plastics, fibre, elastomers and resins). **(03L)**

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

1.3. Introduction to types of polymerization: condensation, addition (cationic and anionic) and copolymerization (without kinetics), chain transfer reactions, Mayo equation of polymerization. **(02L)**

1.4 Techniques of polymerization: Bulk polymerization, solution polymerization, suspension polymerization, emulsion polymerizations, **(03L)**

1.5 Thermodynamics of polymer solutions: Solubility parameter, thermodynamics of mixing**,** theta temperature **(02L)**

Reference Books for Polymer Chemistry:

1. P. Bahadur and N. V. Sastry, Principles of Polymer Science, second edition, Narosa Publishing House, 2005.

2. C. E. Carraher, Jr., Carraher's Polymer Chemistry, 8th edition, CRC Press, New York, 2010.

3. Joel R. 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 Scienc,e A text book,Ane Books Pvt. Ltd,2008.

7 R.Sinha, Outline of Polymer Technology manufacture of Polymers, Prentice hall of India Pvt. 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. Organic Polymer Chemistry, IVY Publishing House,2003.

12 A. Singh, Polymer Chemistry, Campus Book International, 2003.

<u>Books for further reading:</u>

1. ***J. M. G. Cowie, Polymers: Chemistry and Physics of Modern Materials, 2nd ed. (first Indian Reprint 2004), 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 Science, 2nd ed., Kluwer Academic/Plenum Publishers, New York, 2000.***

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

2.1 Micelles and Macromolecules: (08L)

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

2.1.2 Micellization: shape and structure of micelles , hydrophobic interaction, critical micellar concentration (cmc), factors affecting cmc of surfactants, counter ion binding to micelles. (03L)

2.1.3 Solubilization, micellar catalysis ,micro emulsions, reverse micelles, characterization of micro emulsions. (03L)

Reference Books for Surface Chemistry

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.Arun K. Chattopadhyay, Kashmiri Lal Mittal, Surfactants in Solution,Volume 64 of Surfactant Science Series,Volume 64 of Lecture Notes in Pure and Applied Mathematics , illustrated ,Marcel Dekker, 1996

4.K. L. Mittal, American Chemical Society, Micellization, solubilization, and microemulsions, Volume 1
Micellization, Solubilization, and Microemulsions, American Chemical Society, illustrated, Plenum Press, 1977

5.Deepak Thassu, Michel Deleers, Yashwant Pathak, Nanoparticle Drug Delivery Systems
Volume 166 of Drugs and the Pharmaceutical Sciences Series illustrated, CRC Press, 2007

Reference Books

1. K. R. Lange. Surfactants, Hanser Pub. (1999).
2. R. Zana (ed.). Dynamics of Surfactant Self-Assemblies, CRC Press (2005).
3. M. Abe & J. F. Scamehorn. Mixed Surfactant Systems, CRC Press (2004).

2.2 Hydrogen storage by carbon materials: (07L)

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

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

Reference books:

1.Tushar K. Ghosh, Energy Resources and Systems: Volume 2: Renewable Resources,Volume 2 of Energy Resources and Systems, Energy Resources and Systems,SpringerLink : 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, John Wiley & Sons, 2012

4. Yury Gogotsi ,Carbon Nanomaterials, illustratedVolume 1 of Advanced Materials Series,Advanced Materials and Technologies Series,CRC Press, 2006

5.Robert A. Varin, Tomasz Czujko, Zbigniew S. Wronski ,Nanomaterials for Solid State Hydrogen Storage Fuel Cells and Hydrogen Energy illustrated Springer, 2009

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

3.1 Photochemical principles: Environmental effect on absorption and emission spectra, properties of excited states, excited state acidity constants, dipole moments and redox properties. **(04L)**

3.2 Photo physical processes in electronically excited molecules: types of photophysical pathways, types of radiation less transitions, fluorescence emission, fluorescence and structure. triplet state and phosphorescence emission, delayed fluorescence –e type and p-type delayed fluorescence. **(06L)**

3.3 Photochemistry & photochemical reactions of ketones, olefins conjugated olefins and aromatic compounds. **(05L)**

Reference Books for Photochemistry

1 C.H.DePuy, O.L.Chapman, Molecular reactions and photochemistry ,Prentice hall 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 i) collisional quenching, (ii) energy transfer, (iii) electron transfer; examples of (i) pH sensors (ii) glucose sensors (iii) protein sensors. **(05L)**

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

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

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

Reference Books for Fluorescence spectroscopyText 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

PSCHP-302

Paper II

Advanced Instrumental Techniques-I

UNIT-I Spectral Methods – I **(15 L)**

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

1.2 Electron Microscopy: principles, instrumentation and applications of the following:

1.2.1 Scanning Probe Microscopes: (1) Scanning Electron Microscope (SEM),(2) Scanning Tunneling electron Microscope(STEM) and

1.2.2 Atomic Force Microscope(AFM) **(06L)**

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

2.1 Thermogravimetry (TG): Principle and Instrumentation, factors affecting thermogravimetric curves, Interpretation of thermogravimetric curves. applications of thermogravimetry **(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 for Spectral methods –I and thermal methods:

1) **Skoog D A, West D M , Fundamentals of Analytical Chemistry, Thomson Asia Pvt ltd., 8 th Ed, (2004)**
2) **Skoog, Holler, Nieman, Principles of Instrumental Analysis, Thomson Asia Pvt ltd., 5th Ed (2003)**
3) **Sharma B K, Instrumental Methods of Chemical Analysis, Goel Publishing House.**
4) **Wendlandt., Thermal Methods, W W John Wiley,(1986).**
5) **Willard Merrit and Settle, Instrumental Methods of Analysis.**
6) **Douglas A. Skoog, Holler & Crouch , Instrumental analysis India edition CENGAGE Learning (Eighth Indian Reprint 2011)**
7) **Robert D. Braun. Introduction to Instrumental Analysis(Indian Reprint 2006)**
8) **J.W.Dodd, K. Tonge, Thermal Methods. Analytical Chemistry, open Learning.**
9) **Pavia, Lapman, kriz, introduction to Spectroscopy, ThomsonPub.**
10) **H.Straw, &K.walker, Spectroscopy Vol. I&II, Science Paperbacks.**
11) **M.mahindersingh, Analytical chemistry, Instrumental techniques, Dominant Pub. Delhi.**
12) **F.W.fiefield, &D.kealey, Principles and Practice of analytical Chemistry, Blackwell Pub.**
13) ***G.W.Ewing, Instrumnetal methods of Chemical analysis, MacGraw Hill.***

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

3.1Activation analysis- basic principles, fast neutron activation analysis, radio-chemical method in activation 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. Ruticka and J. Stary, Substoichiometry in Radiochemical Analysis, Pergamon Press, (1968)***
2) ***R. A. Faires and G. G. J. Boswell, Radioisotope 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, Nuclear Chemistry, Ane Books Pvt. Ltd. (2009)***
5) ***Nuclear Chemistry By Arnikar***

UNIT-IV Electro-analytical Methods-I (15L)

4.1 Overview of electrode process, Electro-capillary curve and electro-capillary maximum potential. **(02L)**

4.2 Microelectrodes: 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)**

References:

1) ***A. J. Bard and L. R. Faulkner, Electrochemical Methods, 2nd Ed, John Wiley and sons ,Asia Pvt. Ltd, (2004)***
2) ***J. J. Lingane, Electro-analytical Chemistry, 2nd Ed, Interscience 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 Dekkre Inc., New York (A series of volumes)..***
5) ***Donald T. Sawyer, A. Sobkowiak and J. L. Roberts, Jr., Electrochemistry 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, MacGraw hill, 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 electrochemistry, IBH, New Delhi,1990.***

SEMESTER-III

PSCHP-303

Paper-III

Nanochemistry, statistical mechanics & Nuclear chemistry

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

1.1 Variation of optical and magnetic properties of nonmaterial with size, shape, surface characteristics and impurities **(04L)**

1.2 Relationship between size and shape of nanomaterials **(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 polydimethylsiloxane: **(15L)**

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

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

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

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

Reference Books for UNIT-I& II

1. Ludovico Cademartiri and Geoffrey A. Ozin, Concepts of Nanochemistry, Wiley – VCH Verlag GmbH &co, 2009

2.C. Bréchignac, P. Houdy, Marcel Lahmani, Nanomaterials and Nanochemistry, Springer, 2007

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

4.Geoffrey A. Ozin, André C. Arsenault, Ludovico Cademartiri ,Nanochemistry: A Chemical Approach to Nanomaterials ,Royal Society of Chemistry (Great Britain) 2, illustrated ,Royal Society of Chemistry, 2009

Unit- III Statistical Mechanics (15L)

3.1 Distribution of molecules in different states- configuration and weights **(01L)**

***3.2* Thermodynamic probability,** microstates, ensembles, Boltzmann distribution law **(02L**)

3.3 The molecular Partition functions: Translational, rotational, vibrational, electronic and nuclear partition functions. **(03L)**

3.4Statistical Thermodynamics: and Expressions for thermodynamic functions in terms of partition function -Internal energy, the Helmholtz and Gibbs energy, the enthalpy, Heat capacity and equilibrium constants, Sackur –Tetrode equation for the entropy of a mono atomic gas. **(04L)**

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

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

Reference Books for Statistical Mechanics

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

2. John M.Seddon & Julian D. Gale, Thermodynamics and statistical mechanics, Tutorial Chemistry Texts series, Vol.10, Royal society of Chemistry, 2001.

3. Silbey R J & Alberty R A, 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, synchrocyclotron, synchrotron **(04L)**

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

4.3 Nuclear Models**-** Fermi Gas Model, Shell Model, Collective Model, Optical Model **(03L)**

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, radioimmunoassay. **(06L)**

Reference Books for Nuclear Chemistry

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

Semester III

PSCHP-304

Paper IV

Atomic and Molecular: Structure & Spectroscopy

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

1.1 Introduction to approximate methods in Quantum Mechanics- **(06L)**

1.1.1 Variation method linear variation, variation theorem, nonlinear variation,

1.1.2 Perturbation method, first order perturbation

1.2 Calculation of ground state energy and wave function of Helium Atom (Two electron system) using **(07L)**

1.2.1 Variation principle

1.2.2 Pauli's exclusion principle

1.2.3 Slater determinant

1.3 Calculation of wave function for multi electron atoms: **(02L)**

Hartree –Fock self consistent field method,

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

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

2.2 Term symbols, term symbols for He, Li, Be and B atoms **(04L)**

2.3 Exchange 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 , NH_3 ,H_2O, BH_3, CH_4

3.4.2 Huckel molecular orbitals for –ethylene and 1, 3 butadiene and benzene , molecule.

Reference books for Atomic and molecular structure and atomic spectroscopy:

1. ***Laidler and Miser, Physical Chemistry,2nd edition, CBS publishers, New Delhi.(chapters 11-14)***
2. ***Silbey and Alberty ,Physical Chemistry,3rd edition, John Wiley and sons,2000.(Part two quantum chemistry)***
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. Mc Quarrie and J.D. Simon, Physical Chemistry: A Molecular Approach, (1998) Viva Books, New Delhi.***
7. ***J.N. Murrell, S.F.A. Kettle and J. M. Tedder, Valence Theory,2nd edition (1965), John Viley, New York.***
8. ***10 A.K. Chandra, Introductory Quantum Chemistry, 4th edition (1994), Tata McGraw Hill, New Delhi***
9. ***11 D. A. McQuarrie, Quantum Chemistry, Viva Books Private Limited, New Delhi, first Indian ed., 2003.***
10. ***12 R. K. Prasad, Quantum Chemistry, 3rd Ed., New Age International Publishers, 2006.***
11. ***13 James E. House, Fundamentals of Quantum Chemistry, Second Ed., Academic Press, 2005.***
12. ***14 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 polyatomic 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 ofRaman 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 pre-dissociation **(07L)**

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-Hall of India, 2001.**

5. J. Michael Hollas, Modern Spectroscopy, 4th Ed., 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.
5 John P. Lowe, Quantum Chemistry, 3rd ed., Academic Press, New York, 2006.
6 R. Anantharaman, Fundamentals of Quantum Chemistry, McMillan India Limited, 2001.
7 Mahendra R. Awode, Quantum Chemistry, S. Chand and Co. Ltd., New Delhi, 2002.
8 David O. 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, 4th Ed., 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, 3rd Ed., John Wiley and Sons (Asia) Pte. Ltm, 1999.
16 D. C. Harris and M. D. Bertolucci, Symmetry and Spectroscopy, Oxford University.

SEMESTER –IV

PSCHP-401

Paper-I

Chemistry: polymer, green, biophysical and applied.

Unit I: Polymer Chemistry II (15L)

1.1 Identification and characterization of polymers: physical analysis- IR, NMR and ESR spectroscopy, X-ray diffraction analysis, TEM, SEM, ,thermal analysis-TGA, DTA, DSC ,physical Testing -Impact strength, Tensile strength, solubility **(03L)**

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

(01L)

1.3 Properties of polymers: Thermal (glass transition temperature, and its determination), mechanical (deformation and fracture) effects in polymers, viscoelasticity surface properties (surface tension, hardness, friction, abrasion) of polymers, weatherability, rheology and mechanical models, mechanical behaviour. Rubber elasticity. **(03L)**

1.4 Polymer technology: **(04L)**

1.4.1 Polymer auxiliaries, plasticizers, heat Stabilizers, colorants, flame retardants. fillers, reinforcements,

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

1.4.3 Fibers: introduction, production, Fiber spinning, Textile fibers, Industrial fibers, recycling.

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

1.5 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 **(04L)**

UNIT-II Biophysical Chemistry **(15L)**

2.1 Complex Biomolecules of Life: Proteins, enzymes, DNA, RNA, polysaccharides and lipids. chirality and pH dependence of biomolecules. **(02L)**

2.2 Biological significance of physical phenomenon: buffer, micelle, diffusion, osmosis, Donnan membrane equilibrium, viscosity, surface tension, absorption, biosensors : Enzyme based, Electrochemical, immunosensor, fluorescence, optical, Piezoelectric Biosensors . **(02L)**

2.3 Thermodynamics of Biopolymer solutions. Vapour pressure energy and heat of mixing of polymer solution, osmotic, pressure, membrane equilibrium Function and structural basis of classification of muscles, mechanism of muscles, contraction and energy generation. **(04L)**

2.4 Statistical Mechanics in Biopolymer: Chain configuration and confirmation of macro molecule, statistical distribution end to end dimension, calculation of average dimension for various chain structure. **(03L)**

2.5 Electrophoresis (Technique for biomolecular study) : Principle and factors affecting electrophoretic mobility, zone electrophoresis – Paper electrophoresis, cellules acetate electrophoresis, Gel electrophoresis. capillary Electrophoresis, Application of electrophoresis. **(04L)**

Reference Books for Biophysical chemistry

1. U.N Dash,.A Text 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. 0 8Science, 2nd ed., Kluwer Academic/Plenum Publishers, New York, 2000.

Unit III: Polymer &Green Chemistry (15L)

3.1 Polymer Chemistry III (08L)

3.1.1 Engineering and Speciality Polymers: engineering resins, high performance polymers, heat resistant polymers, high impact resistance polymers, speciality polymers, Liquid crystalline polymers, Conducting polymers, Polyelectrolytes, polymers in nonlinear optics. **(03L)**

3.1.2 Applications of polymers in separations, biotechnology and electronics-Membrane Separations, Biomedical Applications, photonic polymers nano-wires, Encapsulation, Electronic shielding., Drag reduction, smart materials, construction and building optical fibers. **(03L)**

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

Reference Books for Polymer Chemistry II & III

Reference Books for Polymer Chemistry:

1. P. Bahadur and N. V. Sastry, Principles of Polymer Science, second edition, Narosa Publishing House, 2005.

2. C. E. Carraher, Jr., Carraher's Polymer Chemistry, 8th edition, CRC Press, New York, 2010.

3. Joel R. 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 Scienc,e A text book,Ane Books Pvt. Ltd,2008.

7 R.Sinha, Outline of Polymer Technology manufacture of Polymers, Prentice hall of India Pvt. 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. Organic Polymer Chemistry, IVY Publishing House,2003.

12 A. Singh, Polymer Chemistry, Campus Book International, 2003.

Books for further reading:

7. ***J. M. G. Cowie, Polymers: Chemistry and Physics of Modern Materials, 2nd ed. (first Indian Reprint 2004), Replika Press Pvt. Ltd.***
8. ***G. S. Misra, Introductory Polymer Chemistry, New Age International (P) Limited, Publishers, 1993.***
9. ***L. H. Sperling, Introduction to Physical Polymer Science. 2nd Edition, John Wiley and Sons. Inc.***
10. ***Hans- Georg Elias, An Introduction to polymer Science, VCH 1997.***
11. ***Charles E. Seymour, Jr., Seymour/Carraher's Polymer Chemistry, 6th ed., Marcel Dekker, Inc., 2003.***

A. Ravve, Principles of Polymer).

3.2 Green chemistry (07L)

3.2.1 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 for Green Chemistry:

1. Mike Lancaster,Green Chemistry An Introductory Text ,Royal Society of Chemistry.

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

UNIT-IV Photochemistry: Kinetics and applications (15L)

4.1. Photophysical Kinetics of bimolecular processes. (07L)

4.1.1 Mechanism of fluorescence quenchin

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 transfermechanis

4.2 Applications of Photochemistry- Importance of photochemistry, origin of life, photosynthesis, mechanism of vision. **((03L)**

4.3 Solar Cells photovoltaic and photo galvanic cells; photo electrochemistry; prospects of solar energy conversion and storage, organic solar cells **(05L)**

Reference Book for Photochemistry

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

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Semester-IV

PSCHP402

Paper-II

Advanced Instrumental Techniques-II

UNIT-I Spectral Methods- II

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 quadrapole resonance spectroscopy, ENDOR, ELDOR, EWDOR (**03L)**

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

2.1 Ion selective field effect transistors, bio-catalytic membrane electrodes, disposable multilayer pIon systems, screen – printed electrodes. **(08L)**

2.2 Chronopotentiometry and chronoamperometry **(05L)**

2.3 Fused salt electrolysis **(02L)**

Reference Books for Unit II & IV

References:

1) ***A. J. Bard and L. R. Faulkner, Electrochemical Methods, 2nd Ed, John Wiley and sons ,Asia Pvt. Ltd, (2004)***
2) ***J. J. Lingane, Electro-analytical Chemistry, 2nd Ed, Interscience 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 Dekkre Inc., New York (A series of volumes)..***
5) ***Donald T. Sawyer, A. Sobkowiak and J. L. Roberts, Jr., Electrochemistry 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, MacGraw hill, 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 electrochemistry, IBH, New Delhi,1990.***
10) ***P.T.Kissinger, W.R. heinman, Laboratoty Techniques in electroanalytical Chemistry, Dekkar, NY. 1984.***

UNIT-III Hyphenated Techniques (15 L)

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, spectro-electrochemistry and radio-chromatography. **(13L)**

Reference Books for Hyphenated Techniques:

1 R.P.W.Scott, Tandem Techniques ,Wiley India Pvt.Ltd. Reprint 2009

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

UNIT-IV Electro-analytical Methods – III (15 L)

4.1 Pulse polarography: 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 K. I. Vasu, Cyclic Voltammetry and the frontiers of Electrochemistry, IBH, New Delhi, (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 Wiley and Sons (Asia) Pvt. Ltd., 2004.***

SEMESTER-IV

PSCHP-403

Paper-III

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 (15 L)

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 metal single crystals, plastic deformation of polycrystalline metals, solid solution strengthening of metals. **(05L)**

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 for Material Science

1. ***William F. Smith, Principles of Material Science and Engineering, 3rd edition, McGraw –Hill Inc.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.***

<u>List of Books for further reading:</u>

1. ***A. R. West, Solid State Chemistry and its Applications, John Wiley and Sons (Asia) Pte. Ltd.,***
2. ***L. E. Smart and E. A. Moore, Solid State Chemistry – An Introduction, 3rd Ed., Taylor and Francis, 2005.***
3. ***V. Raghavan, Materials Science and Engineering, Fifth Ed., Prentice-Hall of India Pvt. Ltd., New Delhi, 2004.***
4. ***William D. Callister, Jr., Materials Science and Engineering, An Introduction, Fifth Ed., John Wiley and Sons (Asia) Pte. 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. Rao and J. Gopalakrishnan, New Directions in Solid State Chemistry, Second ed., Cambridge University Press, 1997.***
9. ***N. B. Hannay, Solid State Chemistry, Prentice Hall of India, New Delhi, 1976.***
10. ***M. Ali Omer, Elementary Solid State Physics, 5th Indian Reprint, Pearson***

Education, Inc., 1999.

Unit III Lasers and superconductors **(15L)**

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

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

3.1.2 Practical lasers- Solid state lasers-Ruby, neodymium, gas lasers-He-Ne, Ar, Kr, Carbon dioxide, Chemical and exciplex Lasers,Dye lasersLED 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 Superconducting solid materials **(05L)**

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

Unit IV Network and Non equilibrium thermodynamics **(15L)**

4.1 Non-equilibrium thermodynamics **(10L)**

4.1.1 Introduction, basic postulates, methodology and rate laws, theorem of minimum entropy production. (03L**)**

4.1.2 Phenomenological coefficients, Curie-Prigogine principle, examples hermoelectricity, electrokinetic phenomena. (04L)

4.1.3 Membrane transport, chemical reactions, applications to biology- entropy production, biological membrane system, Energetic of active transport. **(**03L**)**

4.2 Network Thermodynamics: Introduction, formalism state variables, constitutive relations, bond graph notation, examples- membrane transport, chemical reactions. **(05L)**

<u>Reference Books:</u>

1. ***D. A. McQuarrie and J. D. Simon, Molecular Thermodynamics, Viva Books Private Limited, First Indian Ed., 2004.***
2. ***D. A. McQuarrie and 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, McMillan India Ltd., 2002.***

<u>List of Books for further reading:</u>

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

2. *W. Kauzmann, Thermodynamics and Statistics: with applications to gases, W. A. Benjamin, New York, 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, 3rd ed., Interscience, New York, 1967*

SEMESTER-IV

PSCHP-404

Paper-IV

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 for Symmetry

1 *K.Veera Reddy, Stmmetry and Spectroscopy of molecules,2nd ed, 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 MacGraw hill Pub. Co. Pvt. Ltd.*
5 *P/K. Bhattacharya, Group theory and its chemical applications,1999,Himalaya, Pub. House.*
6 *F.A. Cotton,Chemical applications of Group Theory, Wiley Student Ed., 2006,John Wiley 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 Nuclear Overhauser effect Spectroscopy (NOESY) **(02L)**

2.5 Heteronuclear correlation Spectroscopy (HETCOR) **(02L)**

2.6 Solid-state NMR **(02L)**

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

UNIT-III Spectroscopy **(15L)**

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

3.1.1 Basic principle, hyperfine splitting (isotropic systems); **(02L)**

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 Anisotropic 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 hyperfine splitting, application to study of free radicals spin densities McConnell relationship Zero field splitting. (03L)

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

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

Texts/References:

6. ***C. N. Banwell and E. M. McCash, Fundamentals of Molecular Spectroscopy, 4th Ed., Tata-McGraw-Hill, 1994.***
7. ***M. L. Gupta, Atomic and Molecular Spectroscopy, New Age International Publishers, 2001.***
8. ***H. S. Randhawa, Modern Molecular Spectroscopy, McMillan India Ltd., 2003***
9. ***G. Aruldas, Molecular Structure and Spectroscopy, Prentice-Hall of India, 2001.***
10. ***J. Michael Hollas, Modern Spectroscopy, 4th Ed., John Wiley and Sons, 2004.***

List of Books for further reading:

5. ***R. Drago, Physical Methods for Chemists, Saunders, Philadelphia, 1992.***
6. ***B. P. Straughan and S. Walker (Eds.), Spectroscopy – Vol 1-3, Chapman and Hall, New York, 1976.***
7. ***R. K. Harris, Nuclear Magnetic Resonance Spectroscopy, Pitman, London, 1983.***
8. ***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}H NMR. **(03L)**

4.3 Calculations of chemical shift of hydrocarbons, effect of substituents 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, oxime carbons. **(02L)**

Books Recommended

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,3rd Edition,ELBS,1996.

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.

3. To study the kinetics of the decomposition of hydrogen peroxide in presence of ferric chloride solution and hence to study the effect of the catalyst on the decomposition reaction.

OR

3.To determine the influence of ionic strength on the rate constant for the base catalyzed hydrolysis of ethyl acetate.

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 estimate the amount of a salt of an organic acid/ sparingly soluble salt like magnesium carbonate by ion exchange chromatography.

4 To determine the equilibrium constant for the reaction

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

OR

4To determine the equilibrium constant for the keto- enol tautomerism of ethylacetoacetate.

5 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 potassium ferrocyanide.

pHmetry

1 To 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.

2. To determine the mean ionic activity coefficient of hydrochloric acid by cryoscopy

Colorimetry & spectrophotometry

1 To determine cmc of a dye from its spectral behavior.

OR

1To determine the ionization constant of bromophenol blue.

2 To study the formation of dichromate ion.

OR

2 To study complex formation between nickel (II) with o-phenanthroline.

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

Electroanalytical Methods

1To determine the concentration of lead(II) /cadmium(II) in the given solution by standard addition /calibration curve method.

2To titrate lead(II) with dichromate amperometrically

OR

2 To determine the decomposition potential of copper chloride with copper and platinum electrodes.

Semester –IV

PSCHP4P1

1To determine the formula of the silver (I) ammonia complex by partition method.

OR

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

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

3 To determination of the transport no. of hydrogen ions by moving boundary method.

Non instrumental

1To study the order of the reaction between bromate and bromide.

OR

1 To study the auto catalysis reaction between potassium permanganate and oxalic acid.

.**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.

2To determine ΔG, ΔH and ΔS of dissolution of a sparingly soluble salt by conductometry..

PSCHP4P2

1. To synthesize a polymer and to determine its molar mass by using Ostwald's viscometer.

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

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

Potentiometry

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

OR

1To determine the concentration of chloride ions in the solution by a differential potentiometric titration with solver nitrate..

OR

1 to determine the stability constant of silver(I) ammonia complex potentiometricallly

PSCHP4P3

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

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

pHmetry

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

OR

1 To estimate the amount of a weak base by titration in a non aqueous medium.

Colorimetry & spectrophotometry

1 To determine the rate constant and the order of the reaction for the alkaline hydrolysis of crystal violet

OR

1 To study the kinetics of oxidation of cyclohexanone

2 To study the equilibrium constant for Fe (III) thiocyanate complex.

OR

2 To determine dissociation constant of p-nitro phenol.

PSCHP4P4

1. To study separation of bromocresol green and phenol red by counter current distribution.

2. To study separation of Chromium (III) cationic complexes with ion exchange chromatography

Non instrumental

..**Electroanalytical Methods**

1 To titrate Fe (II) with Ce (IV) biamperometrically.

2 To determine the water content of a sample by Karl Fischer method.

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 of simple polyatomic molecules.
4. Interpretation of NMR, ESR spectra.
5. Interpretation of Mössbauer spectra.
6. Analysis of XRD pattern of cubic system
7. Interpretation of DTA, TG, and DTG curves.

List of reference Books for Practicals:

1. ***B. Vishwanathan and P. S. Raghavan, Practical Physical Chemistry, Viva Books Private Limited, 2005.***
2. ***A. M. James and F. E. Prichard, Practical Physical Chemistry, 3rd ed., Longman, 1974.***
3. ***B. P. Lewitt (ed.), Findlay's Practical Physical Chemistry, 9th ed., 1973.***
4. ***C. D. Brennan and C. F. H. Tipper, A Laboratory Manual of Experiments in Physical Chemistry, McGraw-Hill, 1967.***
5. ***F.Daniel & Others, Experimental Physical chemistry, 19665,Kogakasha Co Ltd. ,Tokyo.***

6. Scheme of examination for M. Sc. Physical Chemistry

7. Semester III and IV.

8. Internal Theory examination (40 Marks)

9.

10. 1**.** One seminar based on curriculum / publication of a research paper/ presentation of a research paper in seminar or conference (to be assessed by teacher of the institution teaching PG learners).
11.
12. A**.** Selection of the topic, introduction, write up, references- **15 marks.**
13.
14. B. Presentation **15 marks.**
15.
16. 2. Active participation in routine class instructional deliveries. **05 Marks**
17.
18. 3**.** Overall conduct as a responsible learner, communication and leadership
19. qualities in organizing related academic activities. **05 Marks**
20.
21. **There will not be any internal examination for practical.**
22.

23. **External Theory Examination (60 Marks)**

Paper	Time allotted in hours	Maximum marks
Paper- I	2.5	60
Paper-II	2.5	60
Paper-III	2.5	60
Paper-IV	2.5	60

24.
25. It is recommended that a total of five questions be set, based on the syllabus with due weight age to the number of lectures allotted per topic. The candidates are expected to answer all five questions. Question 5 will be based on all four units and the remaining questions will be based on the units as indicated below
26.

	Semester- III	Semester-IV
Q.1	Unit-I	Unit-I
Q.2	Unit-II	Unit-II
Q.3	Unit-III	Unit-III
Q.4	Unit-IV	Unit-IV
Q.5	From all four units	From all four units

27.

28. Practicals

29. PSCHPP-3

30. SEMESTER –III

31. 1 The practical examination will be conducted for two days with two sessions per day. Each session will be of 3.5hours duration.

32.

33. 2 The student is expected to complete one major experiment in two sessions. In the remaining two sessions the student will perform two minor experiments one per session.

34. 3 The two minor experiments performed should preferably include one noninstrumental and one instrumental exercise.

35.

36. PATTERN OF EXAMINATION

Semester -III	Session		
Day-I	MORNIBG	MAJOR	Paper-I
	EVENING	MAJOR	Paper-II
DAY-I	MORNING	MINOR- Noninstrumental	Paper-III
	EVENING	MINOR -Instrumental	Paper-IV

37.

38. DISTRIBUTION OF MARKS

39.

	Practical work	Scheme	Viva Voce	Journal	Total		Grand Total
Major	80	05	05	05	95	Paper-I &II	
Minor-I	40	05	05		50	Paper-III	
Minor-II	40	05	05	05	55	Paper-IV	
	160	15	15	10	200		200

40.

Major Experiments		08
Minor Experiments		
	Non-instrumental	05
	Conductometry	02
	Potentiometry	02
	pHmetry	02
	Spectrophotometry	03
	Electroanalytical	02
	Total	16

41.

42. PSCHPP-4

43. SEMESTER-IV

44. 1 The practical examination will be conducted for two days with two sessions per day. Each session will be of 3.5hours duration.

45.

46. 2 The student is expected to complete one major experiment in two sessions. In the remaining two sessions the student will perform one minor experiment in one session and interpretation&calculations of Spectra in the remaining session..

47.

48. PATTERN OF EXAMINATION

Semester -III	Session		
Day-I	MORNIBG	MAJOR	Paper-I&
	EVENING	MAJOR	Paper-II
DAY-I	MORNING	MINOR : Instrumemntal/Noninstrumental	Paper-III
	EVENING	Spectral interpretation&Calculation	Paper-IV

49.

50. DISTRIBUTION OF MARKS

51.

	Practical work	Scheme	Viva Voce	Journal	Total	Paper-I	Grand Total
Major	80	05	05	05	95	Paper-II	
Minor-I	40	05	05	05	55	Paper-III	
Spectral interpretation& Calculation	50					Paper-IV	
	170	10	10	10	200		200

52.

53.

Experiments		
Major Experiments		08
Minor Experiments		
	Non-instrumental	02
	Conductometry	02
	Potentiometry	01
	pHmetry	01
	Spectrophotometry	02
	Electroanalytical	03
	Total	11

Scheme of examination for M. Sc. Physical Chemistry
Semester III and IV.
Internal Theory examination (40 Marks)

1. One seminar based on curriculum / publication of a research paper/ presentation of a research paper in seminar or conference (to be assessed by teacher of the institution teaching PG learners).

A. Selection of the topic, introduction, write up, references- **15 marks.**

B. Presentation **15 marks.**

2. Active participation in routine class instructional deliveries. **05 Marks**

3. Overall conduct as a responsible learner, communication and leadership qualities in organizing related academic activities. **05 Marks**

There will not be any internal examination for practical.

External Theory Examination (60 Marks)

Paper	Time allotted in hours	Maximum marks
Paper- I	2.5	60
Paper-II	2.5	60
Paper-III	2.5	60
Paper-IV	2.5	60

It is recommended that a total of five questions be set, based on the syllabus with due weight age to the number of lectures allotted per topic. The candidates are expected to answer all five questions. Question 5 will be based on all four units and the remaining questions will be based on the units as indicated below

	Semester- III	Semester-IV
Q.1	Unit-I	Unit-I
Q.2	Unit-II	Unit-II
Q.3	Unit-III	Unit-III
Q.4	Unit-IV	Unit-IV
Q.5	From all four units	From all four units