M.Sc. – II

Physical Chemistry

Semester III

Course Code – PSPCH-301

Module – I

1	**Solid State**	15L
1.1	**Point defects**: Point defects in metals and ionic Crystal – Frenkel defect and Schottky defect. Thermodynamics formation of these defects (mathematical derivation to find defect concentration and numerical problems expected); Defects in non-Stoichiometric compounds, colour centres.	06L
1.2	**Line defects**: Edge and Screw Dislocations. Mechanical Properties and Reactivity of Solids.	04L
1.3	**Surface Defects**: Grain Boundary and Stacking Fault. Dislocation and Grain Boundaries, Vacancies and Interstitial Space in Non-Stoichiometric Crystals, Defect Clusters, Interchangeable Atoms and Extended Atom Defects.	05L

Module – II

2	**Atomic spectroscopy**	15L
2.1	Introduction: 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, Term symbols for atoms.	03L
2.2	Exchange interactions and multiplicity of states	02L
2.3	Anomalous Zeeman Effect and Paschen Back effect.	03L
2.4	First order and second order Stark effect in Hydrogen atom, Stark effect in more than one electron system (Helium)	03L
2.5	Atomic spectra and selection rules, energy level diagram of atomic sodium.	04L

Module– III

3	**Molecular Spectroscopy**	15L
3.1	Rotational 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
3.2	Infrared spectroscopy : Harmonic and anharmonic oscillator, vibrational spectra of di and poly atomic molecules, coarse and fine	05L

structure, Nuclear spin effect, application,

3.3 Electronic Spectra of molecules: term symbols for linear molecules, selection rules characteristics of electronic transitions-Franck-Condon principle, types of electronic transitions-d-d, vibrionic, charge transfer, π-π^* , n- π^* transitions, fate of electronically excited states, fluorescence, phosphorescence, dissociation and pre-dissociation — 07L

Module - IV

4 **Group Theory** — 15L

4.1 Recapitulation: point groups, character tables — 02L

4.2 Molecular Orbital Theory of Inorganic Compounds, Symmetry adapted linear combinations, symmetry aspects of MO theory, sigma and pi- bonding for H_2^+,H_2, AB (LiH), AB_2 (BeH_2), AB_3(BH_3), AB_4(CH_4)(tetrahedral, square planner), AB_5 (TBP) AB_6 molecule and bond order. — 09L

4.3 Molecular orbitals for inorganic cage and cluster compounds such as B_6H_6, metal sandwich compounds such as ferrocene and dibenzene chromium. — 04L

References

Module – I

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, 3rd Ed.,Taylor and Francis, 2005.
3. S. O. Pillai, Solid State Physics, Fifth Ed., New Age International Publishers,2002.

Module - II

1. R. K. Prasad, Quantum Chemistry, 3rd Ed., New Age International Publishers, 20
2. Donald A. McQuarrie and John D. Simon, Physical Chemistry-A Molecular Approach, Viva Books PVT Ltd.
3. Peter Atkins and Julio de Paula, Physical Chemistry, 10thEdition, Oxford University Press, Thomson Press (India) Ltd.
4. James E. House, Fundamentals of Quantum Chemistry, Second Ed., Academic Press, 2005.
5. I.N. Levine, Quantum Chemistry, 5 th edition (2000), Pearson Educ. Inc., New Delhi.

Module - III

1. F. A. Cotton, Chemical Applications of Group Theory, 2nd Edition, Wiley Eastern Ltd., 1989.
2. H. H. Jaffe and M. Orchin, Symmetry in Chemistry, John Wiley & Sons, New York, 1966.
3. R. L. Carter, Molecular Symmetry and Group Theory, John Wiley & Sons, New York, 1998.
4. K.V.Reddy, Symmetry and Spectroscopy of Molecules, 2nd Ed., New Age International Publishers, New Delhi, 2009.

Module - IV

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.

Course Code – PSPCH-302

Module – I

1	**Approximate methods in Quantum mechanics**	**15L**
1.1	The Schrodinger equation for Helium atom, Introduction to approximate methods in Quantum mechanics. Variation method, linear and nonlinear variation, secular determinants, Time-independent perturbation theory: nondegenerate and degenerate cases, Introduction to time-dependent perturbation theory. Application to Helium atom in ground state.	10L
1.2	Electron spin, Pauli's exclusion principle, Slater determinant to represent antisymmetricwavefunction.Calculation of wave function for multi electron atoms, Introduction to Hartree –Fockself consistent field method.	05L

Module – II

2	**Molecular Structure**	**15L**
2.1	Born –Oppenheimer approximation, LCAO method- molecular orbital formation, Calculation of ground state energy using Valence bond theory of hydrogen molecule, molecular orbital treatment of H_2^+ ion.	07L
2.2	Construction of hybrid orbital's for equivalent ligand (BeH_2,BH_3,CH_4) to	04L

describe chemical bonding.

2.3 Hückel molecular orbital method for conjugated system (ethylene 1, 3 butadiene, cyclo-butadiene and benzene molecule), Dissociation energy and aromaticity, π electron densities and bond orders. 04L

Module-III

3. **Biophysical** 15L

3.1 Cell membrane and Transport of ions: Permeability of cell membrane, Transport through the cell membrane, passive transport systems, Active transport systems, mechanism of active transport, transport of macromolecules across the plasma membrane, Donnan membrane equilibrium, membrane hydrolysis, Nerve conduction. 03L

3.2 Bioenergetics: Entropy and free energy changes of a biochemical reaction. Endergonic and exergonic processes, coupled reactions, ATP and its role in bioenergetics. 03L

3.3 Statistical Mechanics in Biopolymers: Chain Configuration and Conformation of Macromolecules, Statistical distribution end-to-end dimensions, Thermodynamic probability of chain, Calculation of average dimensions for various chain structures. 03L

3.4 Biopolymer Interactions: Forces involved, Various types of binding processes in biological systems 02L

3.5 Thermodynamics of Biopolymer Solutions: Solutions of biopolymers, Effect of ΔG, ΔH and ΔS on dissolution of a polymer, Entropy and heat of mixing of polymer solutions, Osmotic pressure, Membrane equilibrium, Functional and Structural basis classification of muscles, Muscular contraction, Biochemical activities in muscle contraction. 04L

4 **Statistical Thermodynamics** 15L

4.1 Molecular energy levels, Boltzmann distribution law, partition functions and ensembles, calculation of translational, rotational, vibrational and electronic partition functions, statistical thermodynamics and second law. 07L

4.2 Applications: Calculation of different thermodynamic functions such as internal energy, entropy, free energy, in terms of partition function for mono & di atomic gases , heat capacities of solids ,equilibrium constants,residual entropy, principle of equipartition of energy, Maxwell-Boltzmann, Fermi-Dirac and Bose-Einstein statistics. 08L

References

Module - I and II

1. R. K. Prasad, Quantum Chemistry, 3rd Ed., New Age International Publishers, 20

2. Donald A. McQuarrie and John D. Simon, Physical Chemistry-A Molecular Approach, Viva Books PVT Ltd.
3. Peter Atkins and Julio de Paula, Physical Chemistry, 10th Edition, Oxford University Press, Thomson Press (India) Ltd.
4. James E. House, Fundamentals of Quantum Chemistry, Second Ed., Academic Press, 2005.
5. I.N. Levine, Quantum Chemistry, 5 th edition (2000), Pearson Educ. Inc., New Delhi.

Module - III

1. U.N.Dash, A Text book of Biophysical Chemistry, Macmillan India Ltd.
2. Gurtu and Gurtu, Biophysical Chemistry, PragatiPrakashan.
3. Avinash Upadhyay, KakotiUpadhyay, NirmalenduNath, Biophysical Chemistry:Principles and Techniques, Himalaya Publishers.

Module - IV

1. Donald A McQuarrie, Statistical Mechanics.
2. Thomas Engel and Philip Reid Physical chemistry.
3. Atkins P.W, Physical Chemistry, Oxford University Press, 6th edition, 1998.
4. Leonard K. Nash,Elements of Statistical Thermodynamics: Second Edition.

Semester III
Course Code - PSAIPCH 303

ADVANCED INSTRUMENTAL TECHNIQUES AND SURFACE CHEMISTRY

1	**Module–I: Advanced Instrumental Technique**	**15 L**
1.1	**Mossbauer's spectroscopy**: principle, recoilless emission absorption of gamma rays, experimental methods, instrumentation- drive mechanism, sources, detectors, absorbers effect, calibration of instrument, isomer shift, hyperfine structure (quadruple interactions), magnetic hyperfine interaction, applications, purity and characterization, detection of structurally different atoms in poly nuclear compounds of Iron and Tin	**07 L**
1.2	**Raman Spectroscopy:** theory of excitation of Raman spectra, mechanism of Raman and Rayleigh scattering, comparison of Raman and Infra-red spectra. Intensity of normal Raman peaks, instrumentation, organic and inorganic applications, surface enhanced Raman spectroscopy, resonant Raman spectroscopy, Non-linear Raman	**08 L**

spectroscopy.

2	**Module –II: ESR and Hyphenated techniques**	15 L
2.1	**ESR:** principle, instrumentation, spin-spin splitting, qualitative and multiple resonance (ENDOR, ELDOR) spin labelling, metallic complexes, applications.	07 L
2.2	**Hyphenated techniques**: Need for hyphenation, possible hyphenation, interfacing devices and applications of GC-MS, GC-IR, MS-MS, LC-MS, LC-IR, LC-NMR.	08 L
3	**Module –III: X-ray spectroscopy and thermal methods**	15 L
3.1	**X-ray spectroscopy**: principles instrumentation and applications of X-ray fluorescence, X-ray absorption and X-ray diffraction spectroscopy.	07 L
3.2	**Thermal methods**: principle, instrumentation and applications of: differential thermal analysis (DTA), differential scanning calorimetry (DSC), thermometric titrations, thermo mechanical analysis (TMA), simultaneous thermal analysis (STA), evolved gas analysis (EGA), application in material science.	08 L
4	**Module–IV: Surface Characterization by spectroscopy and microscopy**	15 L
4.1	Introduction to study of surfaces, definition of a solid surfaces, types of surface measurements, general techniques in surface spectroscopy, surface spectroscopic methods, sampling surfaces, surface contaminants.	02 L
4.2	X-ray photoelectron spectroscopy (XPS)	02 L
4.2	Auger electron spectroscopy	02 L
4.2	Basic principle, Instrumentation and applications of Electron microprobe, SEM,TEM and AFM	09 L

References for PSAIPCH 303 (Advanced Instrumental Techniques and Surface Chemistry):

1. Analytical Chemistry, G. D. Christian, 5th Ed. John Wiley, New York (2000)
2. Fundamentals of Analytical Chemistry, D .A. Skoog and D. M. West and F. J. Holler Holt- Saunders 9th Edition (2016)
3. Principles of Instrumental Analysis, D. A. Skoog, F. J. Holler and J.A. Niemann, 8th Edition(1998)
4. Instrumental methods of Analysis, H. H. Willard, L. L. Merritt Jr, J. A. Dean and

F. A. Settle Jr, 7th Ed CBS (1986)
5. Introduction to instrumental analysis, R. D. Braun, McGraw Hill (1987)
6. Wilson and Wilson's Comprehensive Analytical Chemistry, Ed. G. Svehla. (A series of Volumes)
7. Treatise on Analytical Chemistry, Eds I. M. Kolthoff and Others, Interscience Pub. (A series of volumes)
8. Standard Methods of Chemical Analysis, Eds. F. J. Welcher, Robert E. Krieger PublishingCompany, (A series of volumes)
9. Spectroscopy by H Kaur, Prgatiprakashan, 2016.
10. Instrumntal methods of Analysis by Chatwal and Anand, S Chand, 2015

Semester III
Course Code - PSCH 304
NANO CHEMISTRY AND SOME IMPORTANT INDUSTRIAL MATERIALS.

1	**Module - I: Nano chemistry 1:**	**15L**
1.1	Introduction, comparison between bulk and nano materials. Types of nano materials-zero, one, three dimensional nano materials,	**02 L**
1.2	Synthesis of nano materials: Physical methods, Chemical methods and biological methods.	**06 L**
1.3	Properties of nano material with respect to Au, CdSe2, Silica, PolydimehtylSiloxane-mechanical, structural, melting, electrical, optical and magnetic properties.	**07 L**
2	**Module - II: Nano chemistry 2:**	**15L**
2.1	Some important nano materials- carbon nanotubes, porous silicon, mesoporous materials, aerogels, ordered porous materials, self-assembled nano materials and core shell particles.	**09 L**
2.2	Applications of nano martials in electronics, energy, automobiles, sports, textiles, cosmetics, domestic appliances, biotechnology, medical fields and space and research. Environmental effects of nanotechnology.	**06 L**
3	**Module - III: Paints, pesticides and detergents**	**15L**
3.1	**Paints:** Introduction, determination of volatile and non-volatile components, water content of paints, flash point, separation of pigments, binders and thinners of different types, identification and analysis of different types of pigments, organic and inorganic pigments, white tinted and coloured pigments.	**06 L**
3.2	**Pesticides**: Introduction, definition, classification, biodegradation and	**06 L**

	determination of pesticides. pesticide residue analysis, extraction and cleavage of various type of pesticides, use of instrumental method like GLC, TLC, etc.	
3.3	**Detergents**: classification, general scheme of analysis, quantitative method of analysis, active ingredient and equivalent combined SO_3 analysis.	03 L
4	**Module - IV: Petrochemical, explosives, glass and alloys**	15L
4.1	**Petrochemical analysis:** Introduction, definition-fuels, calorific values of fuel, composition and properties of fuels, analysis of petrochemicals, distillation range, moisture content, flash point, fire point, sulphur and carbon residue, doctor test.	04 L
4.2	**Explosives:** definition, heat of explosion, qualitative tests for explosives, quantitative methods for explosive mixtures.	04 L
4.3	**Alloys**: definition, analysis of copper based alloys, aluminium and stainless steel.	03 L
4.4	**Glass**: analysis of different types of glass, soda lime glass, lead glass and borate glass.	04 L

References for PSCH 304 (Nano Chemistry and Industrially important materials)

1. Analytical Chemistry, G. D. Christian, 5th Ed. John Wiley, New York (2000)
2. Fundamentals of Analytical Chemistry, D .A. Skoog and D. M. West and F. J. Holler Holt-
   Saunders 9th Edition (2016)
3. Principles of Instrumental Analysis, D. A. Skoog, F. J. Holler and J.A. Niemann, 8th Edition(1998)
4. Instrumental methods of Analysis, H. H. Willard, L. L. Merritt Jr, J. A. Dean and F. A. Settle Jr, 7th Ed CBS (1986)
5. Introduction to instrumental analysis, R. D. Braun, McGraw Hill (1987)
6. Wilson and Wilson's Comprehensive Analytical Chemistry, Ed. G. Svehla. (A series of
   Volumes)
7. Treatise on Analytical Chemistry, Eds I. M. Kolthoff and Others, Interscience Pub. (A series of volumes)
8. Standard Methods of Chemical Analysis, Eds. F. J. Welcher, Robert E. Krieger PublishingCompany, (A series of volumes)
9. Spectroscopy by H Kaur, Prgatiprakashan, 2016.
10. Instrumntal methods of Analysis by Chatwal and Anand, S Chand, 2015.

11. Concepts of nano chemistry by Cadmitri and others, Wiley publications.
12. Nanotechnology by SulbhaKulkarni, CRC press, 4th edition, 2010

PRACTICALS
Course Code – PSPCHP301 & PSPCHP302
Paper- I and Paper-II
Major Experiments

1. To determine the formula of the copper (II) ammonia complex by partition method.
2. To determine the formula of the zinc (II) ammonia complex by partition method.
3. To determine the van't Hoff's factor by cryoscopy method
4. To determine the molar mass of a non-volatile solute by cryoscopy method.
5. To determination of the transport no. of silver(I) ions by Hittorf's method.
6. To construct the phase diagram for a two-component system forming a compound
7. To construct the phase diagram for a two-component system forming a simple eutectic.
8. To determination of the transport no. of hydrogen ions by moving boundary method
9. To determine the energy of activation and other thermodynamic parameters of activation for the reaction between per sulphate and potassium iodide.

Course Code – PSCHP303
Paper-III

1. To estimate the amount of a salt of an organic acid/ sparingly soluble salt like magnesium carbonate by ion exchange chromatography.
2. To study the order of the reaction between bromate and bromide.
3. To determine the partial molar volume of ethanol
4. To determine the equilibrium constant for the reaction
   $CaSO4\ (s) + 2Ag^{+1}\ (aq) = Ag_2SO_4(s) + Ca^{2+}\ (aq)$
5. To determine the rate constant and the order of the reaction for the alkaline hydrolysis of crystal violet
6. To determine the isoelectric point of gelatine by viscosity measurement.
7. 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.
8. To determine the rate constant and the order of the reaction between per sulphate and iodide ionsby colorimetry.

Course Code –– PSAIPCHP304
Paper-IV

1. To determine the formula of the zinc(II) ferrocyanide complex by titration of Zn(II) sulphate with potassium ferrocyanide.
2. To determine the composition of a mixture of hydrochloric acid, potassium chloride and ammonium chloride by titration with sodium hydroxide and silver nitrate.
3. To determine ΔG, ΔH and ΔS of dissolution of a sparingly soluble salt by conductometry.
4. To determine the stability constant of silver(I) ammonia complex potentiometrically
5. To determine the EO of the quinhydrone electrode.
6. To determine hydrolysis constant and degree of hydrolysis of ammonium chloride and hence to estimate the dissociation constant of the base
7. To determine the ionization constant of bromophenol blue
8. To determine the molar conductance of a weak electrolyte at infinite dilution hence to determine its dissociation constant.

Semester IV

Course Code – PSPCH-401

Module - I

1	**Surface chemistry and Catalysis**	15L
1.1	Micelles and Macromolecules: Surface active agents and their classification, hydrophile- lipophile balance, shape and structure of micelles, critical micelle concentration (cmc), factors affecting cmc of surfactants. Solubilisation and factors affecting solubilisation, micro emulsions, reverse micelles, characterization and applications of micro emulsion	05L
1.2	Fundamentals of adsorption and catalysis: Physical and chemical adsorption-adsorption isotherms, evaluation, chemisorption on metals and metal oxides. Catalysis: concept of activity, selectivity, poisoning, promotion and deactivation. Catalytic kinetics: Concept of Langmuir-Hinshelwood	05L
1.3	Preparation and Characterisation of Catalysts:	05L
1.3.1	General methods of preparation of catalysts: precipitation, sol-gel, hydrothermal, impregnation, hydrolysis, vapour deposition. Activation of catalysts: calcinations, reduction Characterisation of Catalysts: Surface area, pore size distribution, particle size determination, XPS, AES, UV-Vis, FT-IR and thermal methods.	

Module - II

2	**Physical Organic Chemistry and Non-Equilibrium Thermodynamics**	15L
2.1	Physical Organic Chemistry:	08L
2.1.1	Principles of reactivity: Concept of reaction mechanism, Transition state theory, Evaluation of enthalpy of activation(ΔH^*) and entropy of activation(ΔS^*), Mechanistic significance of ΔH^* and ΔS^*, Hammond postulate, Bell-Evans-Polyani principle, Marcus theory.	04L
2.1.2	Solvation and solvent effects: Solvent effect on acid-base reactions, solvent polarity and Hughes-Ingold model, solvent polarity scales, solvent electrophilicity and nucleophilicity, dipolar aprotic solvents.	04L
2.2	Non-equilibrium Thermodynamics:	
2.2.1	Salient features, perspectives and applications of non-equilibrium Thermodynamics. Concepts of entropy production: second law of thermodynamics, entropy production and its rate, entropy production	04L

in closed and open systems.

2.2.2	Onsager's theory and application to chemical reactions: Onsager's reciprocal relations, Uncoupled and coupled reactions.	03L

Module - III

3	**Nuclear chemistry**	15L
3.1	Nuclear fission: types of fission reactions, mass distribution of fission products, emission of neutrons in fission, fissile and fissionable nuclides, theory of nuclear fission, critical energy for fission reactions	04L
3.2	Nuclear Models- liquid drop model, Fermi Gas Model, magic numbers, Shell Model, Collective Model and unified model	04L
3.3	Charged particle accelerator- linear accelerator, cyclotron, Betatron, synchrocyclotron, synchrotron	04L
3.4	Radiation hazards and safety: natural and man-made radiation sources, internal and external radiation hazards, safe handling methods, personal dosimetry, radiation protecting materials	03L

Module - IV

4.	**Advanced Electrochemistry**	15L
4.1	The electrode-electrolyte interface: – The electrical double layer. The Helmholtz-Perrin parallel-plate model, the Gouy-Chapman diffuse-charge model and the Stern model.	4L
4.2	Kinetics of Electrode reactions: Essentials of electrode reactions, Butler Volmmer Model for electrode kinetics, onestep, one electron process through potential energy diagram, standard rate constants and transfer coefficients, equilibrium condition and exchange current, current-over potential equation, facile kinetics and reversible behaviour, introduction to microscopic theories of charge transfer, Marcus microscopic model (derivation expected) The symmetry factor and its significance.	7L
4.3	Applications – Corrosion: Electrochemical corrosion mechanism, short-circuited energy producing cell. Thermodynamics and kinetics of corrosion, methods of prevention of corrosion, Evans diagrams, Potential- pH (Pourbaix) diagrams, Corrosion inhibition by organic molecules. Electrosynthesis – use of electrodes in synthesis of organic compounds.	4L

References

Module - I

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. D.K. Chakrabarty and B.Viswanathan, Heterogeneous Catalysis, Hardcover-October 2008 , New Age International Publishers.
4. B.C. Gates, Catalytic Chemistry, John Wiley and Sons Inc. (1992).

Module - II

1. Addy Pros, theoretical and Physical Principles of Organic Chemistry, John Wiley,1995
2. C. Kalidas and M. V. Sangaranarayan, Non-Equilibrium Thermodynamics,Principles and Applications, McMillan India Ltd., 2002.

Module - III

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.
3. S. Glasstone, Van Nostrand Company ,1967 Sourcebook on atomic energy

Module - IV

1. Allen J. Bard and Larry R. Faulkner Electrochemical Methods: Fundamentals and Applications .
2. John O'M. Bockris and Amulya K.N. Reddy Modern Electrochemistry 1: Ionics, Modern Electrochemistry 2A: Fundamentals of Electrodics ,2nd Edition.

Semester IV
Course Code – PSPCH-402

Module - I

1	**Photochemistry**	15L
1.1	Importance of Photochemistry, Differences between Dark and Photochemical reactions. Physicochemical properties of the electronically excited molecules: Nature of changes on electronic excitation, Crossing of potential energy surfaces, Environmental effect on absorption and emission spectra, properties of excited states, excited state acidity constants, dipole moments and redox properties.	05L
1.2	Photophysical processes in electronically excited molecules: Types of photophysical pathways, Radiation less transitions, Fluorescence emission, Fluorescence and structure, Triplet state and phosphorescence emission, Delayed fluorescence- e type and p-type delayed fluorescence.	05L

1.3	Photophysical kinetics of unimolecular processes and bimolecular processes: Kinetic collisions and Optical collisions, mechanism of fluorescence quenching, Collisions in solution, Kinetics of collisional quenching: Stern- Volmer equation, Deviations from Stern- Volmer equation, Concentration dependence of quenching and excimer formation, quenching by added substances: Charge transfer mechanism, Energy transfer mechanism.	05L

Module - II

2.	**Applications of Fluorescence Phenomena**	15L
2.1	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
2.2	Novel fluorophores: (i) Quantum dots, (ii) lanthanides and (iii) long-lifetime metalligand complexes.	05L
2.3	Radiative decay engineering: metal enhanced fluorescence	03L
2.4	DNA technology –sequencing.	02L

Module - III

3.1	**^{13}C N.M.R. Spectroscopy**	
3.1.1	Elementary ideas, instrumental difficulties, FT technique advantages and disadvantages. proton noise decoupling technique advantages and disadvantages, off-resonance technique	03L
3.1.2	Chemical shifts of solvents, factors affecting chemical shifts, analogy with ^{1}H NMR	02L
3.1.3	Calculations of chemical shift of hydrocarbons, effect of substituents on chemical shifts, different types of carbons (alkene, alkyne and allene), Chemical shift of aromatic carbons and effect of substituent, Chemical shifts of carbonyl, nitrile, oxime carbons	04L
3.2	**Modern nuclear magnetic resonance techniques**	
3.2.1	Spin-relaxation. Nuclear Overhauser Effect (NOE), polarization transfer	02L
3.2.2	Two-dimensional NMR: Correlated spectroscopy (COSY), Heteronuclear correlation Spectroscopy (HETCOR), Nuclear Overhauser effect Spectroscopy (NOESY), Solid-state NMR, Magnetic Resonance Imaging (MRI)	04 L

Module - IV

4.	**Nuclear chemistry (Neutron Activation Analysis)**	15L
4.1	Activation analysis- basic principles, fast neutron activation analysis, radio-chemical method in activation analysis	04L
4.2	Isotopic dilution method- principle and applications	02L

4.3	Auto, x-ray and gamma radiography	04L
4.4	Radiometric Titrations	03L
4.5	Applications of radio-analytical techniques.	02L

References

Module - I

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

Module - II

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

Module - III

1. R. K. Harris, Nuclear Magnetic Resonance Spectroscopy, Pitman, London, 1983.
2. A.E. Derome, Modern NMR Techniques for Chemistry Research, Pergamon, Oxford (1987)
3. Donald L. Pavia, Gary M. Lampman and George S. Kriz, Introduction to Spectroscopy, 3rd ed., Thomson, Brooks/Cole, 2001
4. Organic spectroscopy by William Kemp,3rd Edition, ELBS,1996.
5. J.K.M. Sanders and B.K. Hunter, Modern NMR Spectroscopy, 2 nd edition (1993), Oxford University Press, Oxford. 3. R.K. Harris, Nuclear Magnetic Resonance Spectroscopy, (1986) Addison-Wesley, Longman Ltd., London.

Module - IV

1 J. Ruticka and J. Stary, Substoichiometry in Radiochemical Analysis, Pergamon Press, (1968)
2 H.J.Arnikar, Essentials of Nuclear Chemistry. second. Wiley Eastern Ltd., 1989.
3 R. A. Faires and G. G. J. Boswell, Radioisotope Laboratory Technique, 4th , Ed, Rutterworths; London, (1981)
4 D. Brune, B. Forkman, B. Person, Nuclear Analytical Chemistry, ChartwellBratt Ltd., (1984)
5 Maheshwar Sharon and Madhuri Sharon, Nuclear Chemistry, Ane Books Pvt. Ltd. (2009)

Course Code – PSAPCH 403
Electroanalytical and Polymer Chemistry.

1	**Module - I: Inductively coupled plasma source**	15 L
1.1	Introduction: plasma appearance and spectra, analyteatomisation, ionisation direct current plasma source, plasma source, spectrometers, slew scan spectrometer,	06 L
1.1	Instruments- spectrographs, multichannel, photoelectric spectrometers, arc source emission spectroscopy, characterisation of arc sources,	05 L

	applications	
1.2	Applications: Emission spectroscopy based on arc and sparc source, sample types and sample handling.	04 L
	Module - II: Modern polarographic techniques	15 L
2.1	Recapitulation: classical polarography	02 L
2.2	Cyclic voltammetry	02 L
2.3	Pulse polarography, different pulse polarography, square wave polarography	03 L
2.4	Stripping methods- Anodic and Cathodic stripping methods, Adsorptive stripping methods	04L
2.5	Voltammetry with ultra-microelectrodes	02L
2.6	Biamperometric titrations –Karl Fisher Titrations	02L

Module - III and Module - IV: Polymer

	Module - III: Polymer Synthesis, Properties	15 L
3.1	Polymer science, fundamental terms, historical outline, Classification: Based on origin (natural, semi-synthetic, synthetic), The structure(linear, branched, network, hyper branched, dendrimer, ladder, cross linked, IPN), The type of chain(homo chain, hetrochain), The polymerization mechanism (condensation, addition), the thermal behavior (thermoplastic and thermosetting), the form and application (plastics, elastomers, fiber), Polymer structure; Homopolymers, Copolymers, Tacticity, Geometric Isomerism,	03L
3.2	Molecular Weight and Molecular weight distribution: Average molecularweight,Molecular weight distribution, molecular weight determination by End group analysis, Colligatve property measurement, Light scattering, Ultracentrifugation, Solution viscosity and GPC	03L
3.3	Polymer Synthesis Step-growth Polymerization, Chain-growth Polymerization Polymerization Techniques (Bulk polymerization, solution polymerization, suspension polymerization, emulsion polymerization) Solid state, Gas phase and Plasma Polymerization, Chemical modification , Preparation of polymer Derivatives	07 L
3.4	Polymer Solutions: Criteria for polymer solubility, Thermodynamics of polymer solutions,Solubility parameter, Theta temperature	02L
3.5	Molecular Weight and Molecular weight distribution:	03L

Average molecularweight,Molecular weight distribution, molecular weight determination by End group analysis, Colligatve property measurement, Light scattering, Ultracentrifugation, Solution viscosity and GPC

Module IV: Polymer Structure, Properties, Characterization and Applications 15L

4.1	Solid state properties: Amorphous state, Crystalline state, Thermal transition and properties, Mechanical properties,Visco elasticity and Rubber elasticity	03L
4.3	Polymer Degradation: Thermal degradation, oxidative and UV stability, Chemical and hydrolytic stability, Polymer and environment: Recycling, Incineration, Biodegradation	02L
4.4	**Polymer Technology**	
4.4.1	Polymer Additives, Blends and Composites Additives: Plasticizers, fillers, other important additives. Blends and Composites	02L
4.4.2	Elastomers: Introduction, Types of Rubber, Vulcanization, properties	02L
4.4.3	Fibers: Introduction, Production, Fibre spinning, textile fiber, industrial fiber	02L
4.4.4	Polymer processing: Extrusion, Molding, Calendaring, Coating Polymer Rheology: Non Newtonian flow, Melt instabilities, Drag reduction	02L
4.5	Polymers and advanced Technologies Membrane Science and technology, Bio medical engineering, applications in electronics, photonic polymers	02L

References for Module - I and Module - II

1. Principles of Instrumental Analysis, D. A. Skoog, F. J. Holler and J.A. Niemann, 5th Edition (1998)
2. Instrumental methods of Analysis, H. H. Willard, L. L. Merritt, Jr. J. A.Dean and F. A. Settle Jr 6th Ed CBS (1986)
3. Instrumental methods of Analysis, H. H. Willard, L. L. Merritt Jr, J. A. Dean and F. A. Settle Jr 7th Ed CBS (1986)
4. Introduction to instrumental analysis, R. D. Braun, McGraw Hill (1987)
5. Electrochemical Methods, A. J. Bard and L.R. Faulkner, John Wiley, New YORK, (1980)
6. Electroanalytical Chemistry, J.J .Lingane, 2nd Ed Interscience, New York (1958)

7. Modern Polarographic Methods in Analytical Chemistry, A. M. Bond, Marcel Dekker, New York, 1980.
8. Electroanalytical Chemistry, Ed A. J. Bard and Marcel Dekker, New York, (A series of volumes) 9.Techniques and mechanism of electrochemistry, P. A. Christian and A. Hamnett, Blachie Academic and Professional (1994)
10. Wilson and Wilson's Comprehensive Analytical Chemistry, Ed. G. Svehla. (A series of Volumes)

References for Module - III and Module - IV

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.PolymerScienc,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.

Course Code - PSCH 404
Environmental and Green Chemistry
Environmental chemistry

Module –I: Air and Water Pollution — 15 L

1 **Air pollution:** — 07 L

1.1 Natural and anthropogenic sources of pollution, primary and secondary pollutants, transport and diffusion of pollutants, gas laws governing the behaviour of the pollutants in the atmosphere. — 03L

1.2	Sampling and analysis of: particulate matter, aerosols, SO_2, H_2O, NO_x, CO, NH_3, organic vapours.	O3L
1.3	Effect of pollutants on human beings, plants, animals, materials and on climates.	O1L
	Water pollution:	O8 L
1.4	Sources of water pollution, basic chemistry of water pollutants, effects and control.	O2L
1.5	Determination of water pollution parameters and their significance.	O1L
1.6	Physical parameters: colour, pH, Temperature, odour, turbidity, density, TOS, TSS,TS.	O2L
1.7	Chemical parameters- acidity, alkalinity, hardness, DO, COD, BOD, TOC, THOD, MPN, biological parameters.	O2L
1.8	Heavy metal pollutants like Hg, Pb, Cd, As, Cu, Cr with respect to their sources, distribution, speciation, toxic effect, control, treatment.	O2L
	Module –II: Pollution control technology	15 L
2.1	**Air pollution control technologies:** methods to control air pollution in the environment, Limestone injection and fluidised bed combustion, desulphurisation, catalytic convertor and control of vehicular emission, gravity setting chamber, fabric filters.	O5L
2.2	**Solid Waste disposal**: solid waste disposal methods- open dumps, ocean dumping, land-fills, incineration, recycling and reuse, organic pollutants and hazardous waste disposal and management, non-destructive solid waste, biomedical waste.	O5L
2.3	**Sewage and waste water treatment system**: primary, secondary and tertiary treatments, measurements of treatment efficiencies. biological treatments-aerobic verses anaerobic treatments, bio augmentation and bio stimulation, biofilms in treatments.	O5L
	Module - III: Non renewable energy sources	15L
3.1	Concept and demand of energy, Growing energy needs, Renewable and non renewable sources of energy.	O2L
3.2	Use of alternate energy sources, Wind energy, Solar energy, Nuclear	O6L

energy, Tidal energy. Water as source of energy,.

3.3	Biofuels prodution, use and sustainability, use and over exploitation of energy sources and associated problems	04L
3.4	Role of an individual in conservation of natural resources. Equitable use resources for sustainable lifestyles	03L

Module - IV: Environmental policies, Regulation, Assessment and Green chemistry 15 L

4.1	Important environmental laws in India: Article 48A, Article 51 A, and other laws for environmental management. Role of HOEF and pollution control boards in pollution control- role of international environmental agency- UNEP, GEF, UNFCC and IPCC.	03 L
4.2	Environmental impact assessment (EIM): need of EIA, scope, objectives, types of environmental impacts, steps involved in conducting the EIA studies, techniques- Ad-hoc method, checklist method, overlay mapping method, merits and demerits of EIA studies.	04 L
4.3	Environmental audit: types, objectives, benefits, practice and procedures.	03 L
4.4	Principle and concept of green chemistry, environmental benign solutions, solvent free systems, SCF, ionic liquids as catalysts and solvents, photochemical reactions, chemistry using microwave, sonochemistry, electrochemical synthesis, Designing greener processes- inherently safer designs (ISD), process intensification (PI) in process monitoring. Porous phase reactions, heterogeneous catalysis, bio-catalysis, greener methods.	05 L

References:

1. Environmental Pollution Analysis, S. M. khopkar, New Age International publication(2011).

2. Water and water pollution (hand book) Ed., Seonard'lCiacere, Vol I to IV, Marcel Dekkerinc. N.Y.(1972)

3. Water pollution, Arvindkumar, APH publishing (2004)

4. Introduction to Potable Water Treatment Processes Simon Parsons, Bruce

Jefferson,

Paperback publication.

5. Guidelines for drinking-water quality, third edition, (incorporating first and second addenda). WHO report.

6. Solid waste management, K Sasikumar and SanoopGopi Krishna PHI publication (2009)

7. Solid waste management, SurendrakumarNorthen Book Center (2009)

8. Handbook of chemical technology and pollution control 3rd Edn Martin Hocking AP

Publication (2005).

9. Fundamental Concepts of Environmental Chemistry, Second Edition G. S. Sodhi , AlphaScience, 2005

10. Chemical analysis of metals ; Sampling and analysis of metal bearing ores: AmericanSociety for Testing and Materials 1980 - Technology & Engineering

11. Manual of Procedures for Chemical and Instrumental Analysis of Ores, Minerals, and OreDressing Products. Govt of India Ministry of Steel & Mines, Indian Bureau ofMines, 1979.

12. Alloying: understanding the basics, edited by Joseph R. Davis, ASM Int. (2001).

13. Zone refining and allied techniques, Norman L. Parr, G. Newnes Technology &Engineering (1960).

Sem IV Project for 200 MARKS