M.Sc. CHEMISTRY

PHYSICAL CHEMISTRY SPECIALISATION
SYLLABUS OF III & IV SEMESTERS
REVISED AS PER NEW (CB) SYLLABUS

FOR STUDENTS ADMITTED FROM THE YEAR 2016 ONWARDS

M.Sc. CHEMISTRY (PHYSICAL CHEMISTRY SPECIALISATION)

Syllabus for III and IV Semesters
(for the batches admitted in academic year 2016 & later under CBCS pattern)
[Under Restructured CBCS Scheme]
Grand total marks and credits (all 4 semesters) 2400 marks – 96 credits

(Approved in the P.G. BOS meeting held on 01-07-2017)

Semester - III (Physical Chemistry)
[Under CBCS Scheme]
(for the batches admitted in academic year 2016 & later under CBCS pattern)

	Hrs/week	Internal assessment	Semester exam	Total	Credits
CH(PC)301T (core)	4	20 marks	80 marks	100 marks	4
CH(PC)302T (core)	4	20 marks	80 marks	100 marks	4
CH(PC)303T (Elective)	4	20 marks	80 marks	100 marks	4
CH(PC)304T (Elective)	4	20 marks	80 marks	100 marks	4
CH(PC)351P (LAB-I)	9			100 marks	4
CH(PC)352P (LAB-II)	9			100 marks	4
Total				**600 marks**	**24**

Semester - IV (Physical Chemistry)

	Hrs/week	Internal assessment	Semester exam	Total	Credits
CH(PC)401T (core)	4	20 marks	80 marks	100 marks	4
CH(PC)402T (core)	4	20 marks	80 marks	100 marks	4
CH(PC)403T (Elective)	4	20 marks	80 marks	100 marks	4
CH(PC)404T (Elective)	4	20 marks	80 marks	100 marks	4
CH(PC)451P (LAB-I)	9			100 marks	4
CH(PC)452P (LAB-II)	9			100 marks	4
Total				**600 marks**	**24**

Grand total marks and credits (all 4 semesters) 2400 marks - 96 credits

M.Sc. SEMESTER - III
PHYSICAL CHEMISTRY SPECIALIZATION
(for the batches admitted in academic year 2016 & later under CBCS pattern)

PAPER –CH(PC) 301T: QUANTUM CHEMISTRY AND GROUP THEORY
PC - 09: Applications of Schrödinger equation
PC - 10: Angular momentum & approximate methods
PC - 11: Bonding in molecules
PC - 12: Group theory

PAPER – II CH (PC) 302T : SPECTROSCOPY AND LASERS
PC- 13 : Physical principles of spectroscopy and Vibrational spectroscopy
PC- 14 : NMR , NQR and Mossbaur Spectroscopy
PC- 15 : X-ray Spectroscopy & Diffraction techniques
PC- 16 : Lasers in Chemistry

ELECTIVE 3A
PAPER III CH (PC) 303T(CB1) : APPLIED CHEMISTRY, MATERIAL SCIENCE AND RADIATION EFFECTS
PC(CB1)-1 : Applied kinetics
PC(CB1)-2 : Applied Electrochemistry
PC(CB1)-3 : Types of materials, conducting organics and NLO materials
PC(CB1)-4 : Radiation effects

ELECTIVE–3B
Paper-III CH (PC) 303T(CB2): Biopolymer Chemistry
PC-(CB2)- 5:Bioenergetics and physical properties of biopolymers
PC-(CB2)- 6:Biological membranes and binding of ligands by biopolymers
PC-(CB2) - 7: DNA, genes and cloning
PC-(CB2) - 8: Bioinformatics

ELECTIVE–4A
PAPER-IV CH(PC) 304T(CB3): Polymer Chemistry
PC-(CB3)-9: Polymerization and Kinetics of polymerization
PC-(CB3)-10: Structure and properties of polymers
PC-(CB3)-11: Processing of Polymers
PC-(CB3)-12: Functional polymers

ELECTIVE –4B
Paper IV CH(PC) 304T(CB4): Environmental Chemistry
PC(CB4)-13: Pollution in Atmosphere
PC(CB4)-14: Pollution in Hydrosphere
PC(CB4)-15: Heavy Metal and Radiochemical Pollution.
PC(CB4)-16: Analysis of Air, Water and Metal Pollutants

LABORATORY COURSES

Paper-V CH (PC) 351 P: **Chemical Kinetics**
Paper-VI CH(PC) 352P: Instrumentation

M.Sc. SEMESTER - IV
PHYSICAL CHEMISTRY SPECIALIZATION
(for the batches admitted in the academic year 2016 and later under CBCS pattern)

PAPER-1 CH(PC) 401T(CB1): Thermodynamics, Chemical Kinetics and Electrochemistry
PC- 17.Statistical Thermodynamics
PC- 18. Non-equilibrium Thermodynamics
PC- 19. Chemical Kinetics-II
PC- 20. Electrochemistry –II

PAPER-II CH(PC) 402T: Supramolecular chemistry, Photo Chemistry and Computational chemistry
PC-21 : Supramolecular Chemistry
PC-22 : Photochemistry-II
PC-23 : Computational Chemistry
PC-24: Theoretical treatment of bio polymers

ELECTIVE–3A
PAPER-III CH(PC) 403 T(CB1) : Catalysis
PC-(CB1)-17: Homogeneous catalysis
PC-(CB1)-18: Surface Chemistry and Micellar catalysis
PC-(CB1)-19: Heterogeneous catalysis
PC-(CB1)-20: Phase transfer , Anchored and Photo catalysis

ELECTIVE–3B
Paper IV CH(PC) 403 T(CB2) : Dynamics of chemical reactions and Sensors
PC-(CB2)-21: MO and VB theory of reactivity
PC-(CB2)-22: Kinetic, isotopic, structural, solvent, steric and conformatlonal effects
PC-(CB2)-23:Nucleophilic, electrophilic and free radical reactivity
PC-(CB2)-24: Sensors

ELECTIVE –4A (ID PAPER)
PAPER-IV CH(PC) – 404T(CB3) : Computational Chemistry and It's Applications
PC(CB3)-25: Computational Chemistry – I
PC(CB3)-26: Computational Chemistry – II
PC(CB3)-27: Drug Design Methods I - Ligand Based
PC(CB3)-28: Drug Design Methods II - Structure Based.

ELECTIVE–4B (ID PAPER)
PAPER-IV CH(PC) 404T(CB4): Engineering Chemistry
PC(CB4) -29: Water And Waste Water Treatment
PC(CB4) -30: Corrosion And Its Control
PC(CB4) -31: Energy Sources:
PC(CB4)- 32 Engineering Materials.

ELECTIVE–4C (ID PAPER)
PAPER-IV CH(PC) 405T(CB5): Sugar Chemistry and Sugar Technology
PC(CB5) -33: Advanced Sugar Chemistry
PC(CB5) -34: Sugar and Sugar byproducts
PC(CB5) -35: Methodology used in Sugar Analysis
PC(CB5)- 36: Sugar Technology and Management

LABORATORY COURSES
Paper-V CH (PC) 451P: Chemical Kinetics
Paper-VI CH (PC) 452P: Instrumentation

M.Sc. SEMESTER - III
PHYSICAL CHEMISTRY Specialization
(for the batches admitted in academic year 2016 and later under CBCS pattern)

PAPER –CH(PC) 301T: QUANTUM CHEMISTRY AND GROUP THEORY

PC -09: Applications of Schrödinger equation
PC -10: Angular momentum and approximate methods
PC -11: Bonding in molecules
PC -12: Group theory

PC–09: Applications of Schrödinger equation (15 hrs)

Systems with discontinuity in the potential field. A simple potential barrier. A potential barrier with a finite thickness. Quantum mechanical tunneling – examples - α-particle emission, inversion of NH_3, hydrogen transfer reactions.

The harmonic oscillator – detailed treatment. Wave functions and energies. Vibration of a diatomic molecule – harmonic oscillator model.

The rigid rotator – detailed treatment. Wave functions and energies. Spherical harmonics. Rigid rotator as model for a rotating diatomic molecule.

The hydrogen atom – detailed treatment. Angular and radial functions. Atomic orbitals. Measurability of the ground-state energy of hydrogen atom. Orthonormal nature of hydrogen-like wave functions. Probability calculations.

Atomic and molecular term symbols.
Atoms in external field, Zeeman and anomalous Zeeman effect.

PC–10: Angular momentum and approximate methods (15 hrs)

Angular momentum operators. Commutation relations of angular momentum operators and their consequence. Eigen functions of L^2 and L_z and the eigen values. Magnitude and orientation of angular momentum vectors.

Electron spin. Spin operators. Pauli principle and the Pauli exclusion principle.

Approximate methods- The variation method. Constuction of variation function by the method of linear combinations. H and He atom. Perturbation theory (first order and nondegenerate). Wave function and energy corrections. Application of perturbation theory to the helium atom.
Time- dependent perturbation theory. Interaction of radiation and matter. Allowed and forbidden transitions.

Multielectron atoms. The Hartree-Fock self-consistent field method. Basis functions. Slater-type orbitals (STOs).

PC–11: Bonding in molecules (15 hrs)

Born-Oppenheimer approximation. MO theory of H_2^+ ion. Calculation of MOs and their energies. Evaluation of the overlap integral. Probability curves and enegy diagram. MO theory of H_2 molecule. Calculation of energy. MO theory of polyatomic molecules (general ideas). MO treatment of H_2O. Symmetry-adapted linear combinations. MOs of H_2O.

Concept of hybridization – sp, sp^2, and sp^3 hybrid orbitals.

Semiempirical MO methods. The Huckel theory of conjugated systems. HMO calculations on ethylene, allyl system, butadiene, cyclopropenyl system and benzene. π–electron charges and bond orders. Simplification of secular determinants of cyclopropenyl system, cyclobutadiene and benzene using molecular symmetry. Introduction to extended Huckle Theory, extension of the Huckle's approach to molecules containing heteroatoms.

Orbital symmetry and reactivity: $H_2 + F_2 \rightarrow 2HF$ reaction. $2NO \rightarrow N_2 + O_2$ reaction.

PC–12: Group theory (15 hrs)

Matrices: Addition and multiplication of matrices. Diagonal matrix. Unit matrix. Transpose of a matrix. Adjoint of a matrix. Inverse of a matrix. The determinant of a square matrix. Expansion of a determinant. Properties of determinants.

Symmetry operations forming a group. Classes of symmetry operations. Matrix representation of symmetry operations and point groups. Generation of representations for point groups. Reducible and irreducible representations.

The Great Orthogonality theorem (proof not required) and its consequences. Relation between reducible and irreducible representations. Character tables. Construction of character tables for C_{2h}, C_{2v} and C_{3v} groups.

Quantum mechanics and group theory. Wave functions as bases for irreducible representations. The direct product – vanishing of integrals. Projection operators. Symmetries of vibrations. IR and Raman activity.

Books suggested:

1. Quantum Chemistry, Ira N. Levine, Prentice Hall
2. Introduction to Quantum Chemistry, A. K. Chandra, Tata McGraw Hill
3. Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill
4. Molecular Quantum Mechanics, P. W. Atkins & R. S. Friedman, Oxford University Press
5. Coulson's Valence, R. McWeeny, ELBS
6. The Chemical Bond, J. N. Murrel, S. F. A. Kettle & J. M. Tedder, John Wiley
7. Valency Theory, J. N. Murrel, S. F. A. Kettle & J. M. Tedder, ELBS
8. Chemical Applications of Group Theory, F. A. Cotton, John Wiley & Sons
9. Symmetry and Group Theory In Chemistry, Mark Ladd, Harwood Publishers, London (2000).
10. Symmetry Through the Eyes of a Chemist, I. Hargittai and M. Hargittai, 2nd Edition, Plenum Press, NY (1995).
11. Molecular Symmetry and Group Theory, Robert L. Carter, John Wiley & Sons (1998).
12. Group Theory for Chemists, G. Davidson, Macmillan Physical Science Series (1991).

PAPER – II CH (PC) 302T : SPECTROSCOPY AND LASERS

PC- 13 : Physical principles of spectroscopy and Vibrational spectroscopy
PC- 14 : NMR , NQR and Mossbaur Spectroscopy
PC- 15 : X-ray Spectroscopy and Diffraction techniques
PC- 16 : lasers in Chemistry

PC-13: Physical principles of spectroscopy and Vibrational spectroscopy: (15 Hrs)

Interaction of electromagnetic radiation with matter. Absorption and emission of radiation. Induced absorption, spontaneous emission and stimulated emission. Oscillator strength, transition moment integral. Selection rules, Spectrum of formaldehyde. Factors affecting width and intensity of spectral lines -Line width and natural line broadening, doppler broadening. Intensity of spectral lines.

Infrared spectroscopy- Anharmonic oscillator. Morse potential energy diagram.
Vibration – rotation spectroscopy, P, Q, R branches. Vibration – rotation spectra of polyatomic molecules – linear, symmetric top and asymmetric top molecules. Principles of FTIR.

Raman spectroscopy- Classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrational – rotational Raman spectra. Selection rules. Depolarization factors of Raman lines and their relevance. Instrumentation. Typical applications of Raman spectroscopy – Strucure determination of XY_4 molecules, Phase transitions.

PC-14: NMR, NQR and Mossbaur Specroscopy. (15hrs)

Prnciple of nmr. Derivation of $h\ v = g\ \beta\ H$. Larmor precessional frequency- spin-spin splitting (AX) - Qantitative treatment (proof for J= distance between two successive nmr spectral lines) – Instrumentation - CW instrument and FT instrument.

Two dimensional nmr spectroscopy:
Principles of 2D nmr-Graphical representation of 2D nmr specra – Homonuclear ^1H J, δ spectroscopy-its application for mixture analysis- (for instance mixture analysis of n-butyl bromide and n-butyl iodide) - The COSY experiment. Two dimensional ^1H, ^1H shift correlations. COSY spectra of an AX system, o-nitroaniline, alanine, glutamic acid and arginine.

The nuclear overhauser effect(NOE). wo dimensional nuclear overhauser spectroscopy(NOESY). Nuclear Quadrupole Resonance: Quadrupole nuclei and quadrupole moments-prolate and oblate nuclear charge distributions-energies of quadrupolar transitions-electric field gradient, coupling constants and splitting.

Mossbauer Spectroscopy - Mossbauer effect – Recoil energy, typical Mossbauer spectrum - isomer shift – quadrupole splitting – magnetic hyperfine interaction – ^{57}Fe – Mossbauer spectra of Fe^{2+} and Fe^{3+} (paramagnetic) and Fe^{3+} (magnetic) compounds.

PC-15: X-ray Spectroscopy and Diffraction techniques: (15 hrs)

X-ray fluorescence (XRF) : Experimental method, Processes in X-ray fluorescence, K-emission spectrum of tin, L-emission spectrum of gold.

X-ray absorption: Absorption techniques, Absorption edge fine structure (AEFS spectra) and extended X-ray absorption fine structure (EXAFS) spectra.

X-ray diffraction: Bragg condition. Miller indices, d-spacing formula, Lattice planes and number of d-spacings, experimental methods of X-ray diffraction. Laue method and Debye-Scherrer method. Primitive and nonprimitive unit cells. Indexing the reflections. Identification of unit cells from systematic absences in diffraction pattern. Structure factor and its relation to intensity and electron density. Description of the procedure for an X-ray structure analysis. Typical examples.

Electron diffraction. Scattering intensity versus scattering angle. Wierl equation. Measurement technique. Elucidation of structure of simple gas phase molecules.

PC-16:Lasers in Chemistry: (15 hrs)

General principles of laser action. Stimulated emission. Rates of absorption and emission. Population inversion. Three-level and four-level laser systems. Pumping. Laser cavity – resonant modes. Characteristics of laser light. Laser pulses and their characteristics. Pulse production, Q-switching. Pulse modification, mode-locking.

Practical lasers. Solid-state lasers, gas lasers, chemical and excimer lasers. Examples.

Applications of lasers in chemistry: Femtochemistry. The pump-probe technique. Time-resolved spectroscopy. Photodissociation of ICN. Formation and dissociation of CO-hemoglobin complex. Conversion of ethylene to cyclobutane. Bond selectivity in chemical reactions – the reaction between hydrogen atoms and vibrationally excited HDO molecules.

Lasers and multiphoton spectroscopy – underlying principles. Two-photon spectra of diphenyloctatetraene. Lasers in fluorescence spectroscopy and Raman spectroscopy.

Books suggested:

1. Modern Spectroscopy, J. M. Hollas, John Wiley & Sons
2. Fundamentals of Molecular Spectroscopy, Banwell & McCash
3. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw Hill
4. Molecular Spectroscopy, J. D. Graybeal, McGraw Hill
5. Basic principles of Spectroscopy, R. Chang, McGraw Hill
6. Physical Methods for Chemistry, R. S. Drago, Affiliated East West Press
7. Vibrational Spectroscopy: Theory and Applications, D. N. Sathyanarayana, New Age International
8. Introduction to Raman Spectroscopy, J. R. Ferraro & K. Nakamoto, Academic Press
9. NMR Spectroscopy: Basic principles, concepts and applications in chemistry, H. Gunther, John Wiley-VCH publishers
10. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R. V. Parish, Ellis Harwood
11. NMR basic principles - Atta-ur-Rahman, Springer.
12. Two dimensional NMR Spectroscopy-Applications for chemists and biochemists, edited by W. R. Croasmun & R. M. K. Carlson, Wiley-VCH
13. X-ray diffraction procedures for polycrysralline and amorphous materials, H. P. Klug & L. E. Alexander, John Wiley
14. Physical Chemistry, Ira N. Levine, McGraw Hill
15. Atkin's Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press
16. A Guide to Lasers in Chemistry, G. R. Van Hecke & K. K. Karukstis, Jones and Bartlett Publishers
17. Lasers in Chemical and Biological Sciences, S. Chopra & H. M. Chawla, Wiley Eastern Ltd.
18. Molecular structure and Spectroscopy, G.Aruldas, Eastern Economic Edn.

ELECTIVE 3A

PAPER III CH(PC) 303T(CB1) : APPLIED CHEMISTRY, MATERIAL SCIENCE AND RADIATION EFFECTS

PC(CB1)-1 : Applied kinetics
PC(CB1)-2 : Applied Electrochemistry
PC(CB1)-3 : Types of materials, conducting organics and NLO materials
PC(CB1)-4 : Radiation effects

PC(CB1)-1:Applied kinetics (15 hrs)

Kinetics and chemical reaction engineering. Reactor design: Basic objectives in design of a reactor. Parameters affecting the reactor performance. Balance equations for reactor design. Single ideal reactor models.

Batch reactors (BR): General features. Design equations for a BR. Material and energy balances. Isothermal operation, constant-density system.

Continuous stirred-tank reactors (CSTR): General features. Design equations for a CSTR. Material and energy balances. Constant-density system. Steady-state operation at specified temperature. Damkohler number – numerical problems.

Plug-flow reactors (PFR): General features. Design equations for a PFR. Material and energy balances. Constant-density system.

Comparisons of ideal reactors for a single reaction. Single-vessel comparisons. BR and CSTR. BR and PFR. Numerical examples.

PC(CB1)-2:Applied Electrochemistry (15 hrs)

Batteries: Battery parameters. Energy density power density and Ragone plot. Measures of battery performance. Primary and secondary batteries. Zn/MnO_2, lead-acid and Ni-Cd batteries and Lthium cells; Lithium-thionylchloride cell and lithium-ion battery.
Fuel cells: General Chemistry of Fuel cells. Types of fuel cells: H_2/O_2 and methanol/O_2 fuel cells. Use of porous electrodes in fuel cells. Advantages, limitations and efficiency of fuel cells.

Photovoltaic cells: Semiconductor based photoelctrochemical cells. Electrochemical energy from solar energy.

Anodic oxidation of metals. Characteristics of anodic oxide films. Industrial application of anodic oxide films.

Electroplating: Technical importance. Mechanism of electroplating. Alkaline and acid plating of copper, nickel.

Electro-organic synthesis: Reduction of carboxylic acids, the polymerization of acrylonitrile to adiponitriles in the synthesis of nylon. Reduction of nitro compounds.

PC(CB1)-3:**Types of materials, Conducting Organics and NLO materials** (15 hrs)

Classification of materials – metals, ceramics, polymers, composites, semiconductors and biomaterials.

Glassy state – glass formers and glass modifiers, applications
Ceramics – criteria for determining the crystal structure of ceramic materials – examples.
Composites – particle reinforced and fibre reinforced composites.

Preparative methods of solid materials - Ceramic method (Solid State method), co-precipitation as a precursor to solid state reaction, solutions and gels (Zeolite synthesis), crystallization from melts: Czochralski method, Kyropolous method; vapour phase transport method, modification of existing structure by ion-exchange and interaction reactions.

Techniques of single crystal growth – growth from solutions – growth from melts – growth from vapour. Non-linear optical (NLO) behavior– basic concepts, second and third harmonic generation, examples of organic, inorganic and polymer NLO materials.
Conducting organics – Fullerenes, alkali metal doped fullerides, fullerenes as superconductors

PC(CB1)-4: Radiation effects 15hrs

Radiation hazards and safety: Radiation effects. High-energy radiation and high-energy particles – types and sources. Radiation protecting materials.
Radiation chemistry of liquid water. Chemical yields. Dosimetry. Fricke dosimeter and thiocyanate dosimeter. Effect of radiation on DNA. Direct and indirect effects. Reaction of OH radicals with DNA constituents. General mechanism of strand break formation in DNA by OH radicals.

Radioactive wastemanagement: Introduction, Classification of radioactive waste, Treatment of Radioactive waste: Radioactive waste disposal.

Applications of radioisotopes in nuclear medicine and pharmaceuticals: general applications of radiopharmaceuticals, use of nuclear properties of indicator nuclides. In vivo diagnostic procedures, in vitro diagnostic testing therapeutic use of radiations, Use of radiation for food preservation and sterilization.

Books suggested:

1. Introduction to Chemical reaction Engineering and Kinetics, R. W. Missen, C. A. Mims & B. A. Saville, John Wiley
2. Chemical Reaction Engineering, O. Levenspiel, John Wiley
3. Chemical Engineering Kinetics, J. M. Smith, McGraw Hill
4. Elements of Chemical Reaction Engineering, H. Scott Fogler, Prentice Hall (page-114)
5. Modern Electrochemistry 2B, Bockris & Reddy, Plenum
6. Industrial Electrochemistry, D. Pletcher, Chapman & Hall
7. Introduction to Electrochemistry, S. Glasstone, EAST-WEST Press Pvt. Ltd, New Delhi
8. Electrochemistry – B K Sharma
9. Fundamental principles of Modern Electroplating, Lowenheim, John Wiley
10. The physics and chemistry of solids. Stephen Elliot, John Wiley & Sons
11. Solid state chemistry and applications. A.R.West, John Wiley & Sons

12. New directions in solid state chemistry. CNR Rao and Gopalakrishnan, Cambridge University Press
13. Principles of the Solid State, H. V. Keer, New Age International
14. Material Science and Engineering – An Introduction, William D. Callister, Jr., Wiley & Sons
15. Materials Science & Engineering – A First Course, V. Raghavan, Prentice Hall
16. Radiation Chemistry: Principles and Applications, Farhataziz and M. A. J. Rodgers (Eds.), VCH Publishers, New York (1987).
17. Radiation Chemistry: Present Status and Future Trends, C. D. Jonah and B. S. M. Rao (Eds.) Elsevier, Amsterdam (2001).
18. Essentials of Nuclear Chemistry: H. J. Arnikar. New Age Publication Ltd. (1995).
19. Radiation chemistry and Nuclear Methods of Analysis W. D. Ehmann, D. E. Vance. John Wiley (1991).
20. Nuclear and Radiochemistry G. Friedelarder, J. W. Kennedy, E.. S. Macias, J. M. Miller John Wiley (1981).
21. Source Book of Atomic Energy, S. Glasstone, D. Van Nostrand (1967)
22. Nuclear analytical chemistry- J. Tolgyessy and S. Verga Vol. 2 , University park press (1972)
23. Fundamental of Radiochemistry, D.D.Sood, A.V.R.Reddy, N.Ramamoorthy, IANCAs , Mumbai, 4th Edition

ELECTIVE –3B

Paper III CH(PC) 303T(CB2) : BIOPOLYMER CHEMISTRY

PC(CB2)-5: Bioenergetics & physical properties of biopolymers
PC(CB2)-6: Biological membranes & binding of ligands by biopolymers
PC(CB2)-7: DNA, genes and cloning
PC(CB2)-8: Bioinformatics

PC(CB2)-5: Bioenergetics and physical properties of biopolymers (15 hrs)

Bioenergetics: The standard state in biological processes. ATP – the currency of energy. Gibbs energy change in ATP hydrolysis, comparison with other phosphates. Principles of coupled reactions. Glycolysis and coupled reactions involving ATP. Biological oxidation-reduction reactions – transfer of H^+ ions and electrons. Synthesis of ATP in the mitochondria. The chemiosmotic theory. Gibbs energy change accompanying the proton movement.

Viscometry: Molecular weights. Use of viscometry in the study of ligand binding to DNA. Separation/molecular weight studies of biopolymers.Light scattering method.

Sedimentation: Sedimentation velocity. Sedimentation coefficient. The Sverdberg equation. Sedimentation equilibrium analysis. Ultra centrifugation Molecular weights. Light scattering method.

Electrophoresis : principle involved. Gel electrophoresis. Electrophoretic mobility. Applications.

PC(CB2)-6: Biological membranes and binding of ligands by biopolymers (15 hrs)

Structure and function of cell membrane. Membrane equilibria and thermodynamics of membrane equilibria. Dialysis equilibrium. Osmotic pressure. Membrane potentials. Transport across membranes. Passive transport, facilitated transport and active transport.

Sodium-potassium pump. Selective ion transport and membrane potential. The Goldman equation (derivation not required). Nerve cells. The transfer of information in the body. The action potential and the mechanism of action potential propagation. Signal transducing mechanism involving gated ion channels in the plasma membrane.
Binding of ligands and metal ions to macromolecules – one and n-euqivalent binding sites per molecule. Allosteric interactions – Oxygen binding to myoglobin and hemoglobin – Cooperative and non-cooperative binding. Hill equation and Hill plots. Transport of H^+ and CO_2 . Bohr effect.

PC(CB2)-7: DNA, genes and cloning (15 hrs)

Watson –Crick model of DNA. Types of DNA chains – linear, circular and supercoiled DNA. Types of RNA. Secondary structure of t-RNA

Genes and genome. Gene expression. Transcription and translation (general principles only). Codons and the genetic code. Sequence analysis of DNA by the Sanger chain-termination method.
Introduction to biotechnology and recombinant DNA technology. Molecular cloning. Restriction endonucleases and cloning vectors. Steps involved in the construction of recombinant DNA. DNA hybridization and hybridization probes.

Satellite DNAs – micro and mini satellites. Sequence polymorphisms – RFLPs. Principles of DNA finger printing technology.

PC(CB2)-8: Bioinformatics (15 hrs)

Introduction: Use of informatics and computers in biology. Homology as descendants of common ancestors, statistical analysis of sequence alignment.

General purpose Databases for Comparative Genomics: COGs, KEGG, MDGB -
Organism Specific Databases examples - E. Coli, Yeast, Oryza.

Introduction to Proteins - primary, secondary, tertiary and quaternary structures.

Structure databases – PDB, MMDB, CSD. Homology modeling – Flow chart, structure refinement - Ramachandra Plot.

Books suggested:

1. Biophysical Chemistry, Cantor & Schimmel, W. H. Freeman and Company
2. Principles of Physical Biochemistry, Kensal E van Holde, W. Curtis Johnson & P. Shing Ho, Prentice Hall
3. Physical Biochemistry : Principles and Applications, David Sheehan, John Wiley
4. Physical Chemistry for the Chemical and Biological Sciences, Raymond Chang, University Science Books
5. Lehninger Principles of Biochemistry, D. L. Nelson & M. M. Cox, MacMillan
6. Biochemistry, L. Stryer, W. H. Freeman and Company
7. Concepts in Biochemistry, Rodney Boyer, Books/Cole Publishing Company
8. Modern Electrochemistry 2B, Bockris & Reddy, Kluwer Academic/ Plenum
9. Introduction to Bioinformatics by Arthur Lesk, Oxford University Press, Inc, New York
10. Bioinformatics, A practical guide to the Genes and Proteins. Edited by Andreas. D. Baxevanis and B. F. Francis Wiley Publishers

ELECTIVE 4A

Paper IV CH(PC) 304T(CB3) :POLYMER CHEMISTRY

PC(CB3)-9: Polymerization and Kinetics of polymerization
PC(CB3)-10: Structure and properties of polymers
PC(CB3)-11: Processing of Polymers
PC(CB3)-12: Functional polymers

PC(CB3)-9: Polymerization and Kinetics of polymerization (15 hrs)

Classification of polymers. Types of polymerization.

Kinetics and mechanism of free radical polymerization. Degree of polymerization, kinetic chain length and chain transfer coefficient – Trommsdorff effect. Effect of pressure and temperature on chain polymerization.

Kinetics and mechanism of cationic, anionic polymerization, coordination polymerization, linear stepwise polymerization.

copolymerization reactions and copolymer composition. Reactivity ratios and their determination. Alfrey and Price Q-e scheme for monomer and radical reactivity. Block and graft copolymers.

Polymerization in homogeneous and heterogeneous systems. Techniques of polymerization-Bulk, solution, suspension and emulsion polymerizations.

PC(CB3)-10: Structure and properties of polymers (15 hrs)

Polymer solutions:

The process of polymer dissolution. Thermodynamics of polymer dissolution. Entropy, heat and free energy of mixing of polymer solutions. Conformations of dissolved polymer chains. The freely jointed chain. Short-range and long-range interactions. The Flory-Huggins theory of polymer solutions. Dilute polymer solutions. Flory-Krigbaum theory.

Mechanical properties of polymers:

The elastic state. Rubber-like elasticity and viscoelasticity. Newtonian and non-Newtonian behaviour. Maxwell and Voigt-Kelvin models of viscoelastic behaviour.

The crystal structure of polymers. Morphology of crystalline polymers. Crystallization and melting. Determination of Tm. Thermodynamics of crystalline melting. Heats and entropies of fusion. Degree of crystallinity. Factors affecting the crystallization.

The glassy state – glass transition temperature Tg of polymers. Factors influencing Tg. Glass transition temperature and melting point.

Molecular weight distribution – measurement of molecular weights by end group analysis, osmometry and GPC.

PC(CB3)-11: Processing of Polymers (15hrs)

General applications of Polymers. Polymer Additives - Fillers, plasticizers, lubricants, catalysts, stabilizers, colorants, antioxidants, flame retardents.

Processing techniques of polymers - one dimensional coating -Adhesives, Lamination; extrusion- calendering and thermoforming ; Molding of Polymers- Process, advantages and limitations of Compression molding, Injection Molding, Extrusion Molding, Blow Molding.

Casting - Types, Vacuum Casting, Potting, Encapsulation, Film Casting,.

Fibre Reinforced Plastics- preparation and properties. Synthetic Fibres- Rayons, (Nitro cellular, Cupammonium, Diacetate, Viscose), Nylons, Dacron.

Processing of fiber reinforced Composites- Pultrusion technique, prepreg production processes, filament winding.

PC(CB3)-12: Functional polymers (15hrs)

Smart materials – Their uses in sensing devices and in communication networks.

Electrically conducting polymers- Introduction, basic principles and their applications. Brief description of polyanilines, polypyrrole, polyacetylene and polythiophene.

Photoconductive polymers, Liquid crystal polymers – smectic, nematic and cholesteric structures, Ionic exchange polymers- Cationic and anionic exchange polymers and their uses.

Biodegradable polymers- Definition, classification, applications. Brief description of polyhydroxyalkanoates, polycaprolactone, polyacetic acid and polyvinylalcohol.

Polymers in Membrane separation. Filtration – micro, ultra and nanofiltration. Separation of gases – permeselectivity and gas permeability of representative polymers. Liquid separation – dialysis, electro osmosis and reverse osmosis.

Fire retarding polymers, photonic polymers.
Polymers in biomedical applications – artificial organs and controlled drug delivery.

Books suggested:

1. Textbook of Polymer Science, F. W. Billmeyer Jr, John Wiley & sons
2. Polymer Science, V. R. Gowarikar, N. V. Viswanathan & J. Sreedhar, Wiley Eastern
3. Contemporary Polymer Chemistry, H. R. Alcock & F. W. Lambe, Prentice Hall
4. Physics and Chemistry of Polymers, J. M. G. Cowie, Blackie
   Academic and professional
5. Materials scince and engineering an introduction by William D Callister, Jr. Wiley Publishers
6. Polymer Chemistry, B. Vollmert, Springer publishers
7. Physical Chemistry of Polymers, A. Tagers, Mir Publishers
8. A text book of polymers, Vol. I,II,III, M.S. Bhatnagar, S. Chand publishers

ELECTIVE 4B

Paper IV CH(PC) 304T(CB4) : ENVIRONMENTAL CHEMISTRY

PC(CB4)-13: Pollution in Atmosphere
PC(CB4)-14: Pollution in Hydrosphere
PC(CB4)-15: Heavy Metal and Radiochemical Pollution.
PC(CB4)-16: Analysis of Air, Water and Metal Pollutants

PC(CB4)-13: Pollution in Atmosphere

Typical Composition of Unpolluted Dry Air - Major Air Pollutants: Carbon Monoxide, Nitrogen Oxides, Sulphur Oxides, Particulate Matter, Hydrocarbons, Chloroflurocarbons.

Carbon Monoxide: Sources and Sinks, Concentration Profile, Effects on Human Health, Control of CO Emissions.

Nitrogen Oxides (NO_x): Reactions Leading to Formation of NO_x, Sources and Sinks, Concentration Profile, Harmful Effects of NO_x on Human Beings, Plants, Materials and Control of NO_x Emissions.

Sulphur Oxides (SO_x): Reactions Leading to Formation of SO_x, Sources of SO_x. Harmful Effects on Human Beings, Plants and Materials - Control of SO_x Emissions - Acid Rain: Formation and Toxic Environmental Effects.

Particulate Matter: Sources, Inorganic and Organic Particulate Matter - Effects on Human Beings, Materials and Climate - Control of Particulate Emissions.

Hydrocarbons: Sources - Types of Polluting Hydrocarbons - Hydrocarbons and Photochemical Smog Formation - Harmful Effects of Photochemical Smog - Control of Hydrocarbon Emissions .

Green House Effect: Causes, Consequences and Abatement of Green House Effect - Ozone Depletion - Mechanism, Causes, Consequences and Abatement of Ozone Depletion - Bhopal Gas Tragedy and Sevozo Disaster.

PC(CB4)-14: Pollution in Hydrosphere

Types of Water Pollutants and their Effects - Sources of Water Pollution: Domestic, Industrial, Agricultural, Soil, Thermal and Radioactive Wastes - Types of Persistent Pollutants - Biomagnification of Persistant Pollutants, Effects of Biomagnified Pollutants on Human Beings (DDT) – Tripolyphosphates: Their Role in Eutrophication of Water Bodies - Ecological Consequences of Eutrophication, Bacteriological Contamination of Water - Dissolved Oxygen in Natural Waters - Depletion of Dissolved Oxygen - Biological Oxygen Demand and Chemical Oxygen Demand as Indicators of Extent of Water Pollution - Nitrates, Nitrites, Nitrosoamines in Water: Their Toxic Effects On Human Beings - Treatment of Drinking Water Supplies.

PC(CB4)-15: Heavy Metal and Radiochemical Pollution.

Essential and Toxic Elements in Nature - Mechanism of Metal Ion Toxicity - Effects on Non-Metalloenzymes, Metalloenzymes, Cell Membranes, Nucleic Acids - Concepts of Speciation, Biomethylation and Biomagnification.

Mercury: Sources of Pollution. Speciation and Environmental Forms of Mercury - Biochemical Effects of Different Species of Mercury - Minamata Bay Episode as a Case Study of Mercury Poisoning.

Arsenic: Sources of Pollution - Speciation and Environmental Chemistry of Arsenic - Biochemical Effects of Different Species of Arsenic.

Lead: Sources of Lead Pollution - Speciation and Pathways of Lead in Environment - Biochemical Effects of Lead.

Cadmium: Sources of Pollution – Speciation - Biochemical Effects of Cadmium Poisoning.
Radiochemical Pollution: Sources, Chemical Changes due to Radiation on Water.

Organic Compounds - Harmful Effects of Radioactive Pollutants on Living Organisms - Permissible Limits of Radiation - Control and Disposal of Radioactive Wastes - Chernobyl Disaster.

PC(CB4)-16: Analysis of Air, Water and Metal Pollutants

Air Quality Standards - Sampling (Particulates and Gaseous Pollutants) - Analysis of Pollutants: SO_2 (Modified West-Gaeke Spectrophotometric Method, Pulsed Fluorescence Spectrometry), H_2S (Spectrophotometry – Ethelyne Blue Method), NO-NOx (Chemiluminescence Technique, Colorimetric Technique- Saltzman Method) – CO (NDIR Spectrometry, GC), Hydrocarbons (Ionization Analysis), Aromatic Hydrocarbons in Automobile Exhausts, Petrol, Air, O_3 (Chemiluminiscene and Spectrophotometry) - Particulate Matter Analysis (High Volume Method).

Water Sampling, Preservation and Preconcentration Methods and Physical Analysis - Colour, Odour, Temperature, pH, EC, Redox Potential and Total Dissolved Solids (Turbidimetry). Chemical Analysis of Anions: CN^-, Cl^-, F^- (Spectrophotometry, Ion Selective Potentiometry and Titrimetry), NO_2^- and NO_3^- (Spectrophotometry), SO_4^{2-}, PO_4^{3-}, HCO_3^-, CO_3^{2-}, Hardness of Water (Titrimetry), Ammonical Nitrogen (Spectrophotometry) - Determination of DO, BOD, COD, TOC in Water.

Books Suggested:

1. Environmental Chemistry, John. W. Moore and Elizabeth Moore Academic press New York
2. Principles of Environmental Chemistry, Stanley E. Manahan 2nd Ed.
3. Environmental Chemistry, 4th ed. A.K. De. New Age International Publishers, 2000
4. Environmental Pollution Analysis, S.M. Khopkar Wiley Eastern Ltd. 1995
5. Environmental Chemistry, Colin Baird W.H. Freeman and Company New York 1995.
6. Text Book of Environmental Chemistry, Ayodhya Singh, Campus Books International publishers
7. Chemistry of the Environment, II Edn Thomas G.Spiro William M.Stigliani
8. Fundamental Concepts of Environmental Chemistry, G.S.Sodhi Narosa Publishing House.
9. Environmental Analytical Chemistry, F.W.Fifield,P.J.Haines,Blackie Academic & Professional

III SEMESTER PRACTICALS

CH (PC) 351 P: Paper-V (Chemical Kinetics) **9** hrs/week

Note: The data obtained in all the experiments are to be analyzed by the students both *by the usual graphical methods and by regression (linear/nonlinear) techniques using a PC.*

- Study of peroxydisulphate – iodide reaction:
  1. Individual orders of the reactants by initial rate and isolation methods
  2. Effect of temperature on reaction rate
  3. Effect of ionic strength on reaction rate
- Study of peroxydisulphate – iodide clock reaction:
  1. Individual orders of the reactants ,
  2. effect of ionic strength on uncatalyzed and Cu(II)-catalyzed reactions
- Study of acetone – iodine reaction by titrimetry
  1. Order w.r.t.[iodine]
  2. Order w.r.t. [acetone]
  3. Order w.r.t. [H+]

CH (PC) 352 : Paper-VI (Instrumentation) 9 hrs/ week

Conductometry:

- Conductometric titrations:
  1. Mixture of strong and weak bases vs strong acid
  2. Mixture of strong and weak acids vs weak base
  3. Mixture of strong acid, weak acid and CuSO4 vs strong base
  4. Mixture of halides (chloride + iodide) vs AgNO3
  5. Formic acid, acetic acid, chloroacetic acid, dichloroacetic acid and Trichloroacetic acid
  6. and their mixtures vs strong base
  7. Precipitation titration: K2SO4 vs BaCl2
- Dissociation constants of weak acids
- Effect of solvent on dissociation constant of a weak acid
- Verification of Onsager equation
- Composition of Cu(II) – tartaric acid complex by Job's method

pH metry:

- pH – metric titrations:
  1. Monobasic acids vs strong base
  2. Dibasic acid vs strong base
  3. Tribasic acid vs strong base
  4. Mixture of strong and weak acids vs strong base
- Determination of dissociation constants of monobasic/dibasic acids by Albert- Serjeant method
- Determination of dissociation constant of acetic acid in DMSO, acetone anddioxane
- Determination of pKa and pKb of glycine (calculation using a computerprogram)
- Determination of stability constant of a metal complex

Suggested books:

1. A textbook of practical organic chemistry by A I Vogel, Vol 1&2.
2. Senior practical physical chemistry. B. D. Khosla, V.C. Garg, Adarsh Gulati
3. Experimental Physical Chemistry: V. Athawale and P. Mathur.
4. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.
5. Practical in Physical Chemistry: P.S. Sindhu
6. Advanced Practical Physical chemistry: J.B.Yadav

M.Sc. SEMESTER - IV
PHYSICAL CHEMISTRY SPECIALIZATION
(For the batches admitted in academic year 2016 and later under CBCS pattern)

PAPER I CH(PC)401: Thermodynamics, Chemical kinetics and Electrochemistry

PC-17 : Statistical Thermodynamics
PC-18 : Non-equilibrium Thermodynamics
PC-19 : Chemical Kinetics-II
PC-20 : Electrochemistry -II

PC -17: Statistical Thermodynamics (15 hrs)

Concepts of distribution and probability. Estimation of probability and the most probable distribution. Systems composed of noninteracting particles. Derivation of Boltzmann distribution law. The molecular partition function. Systems composed of interacting particles.

The concept of ensemble and canonical ensemble. Canonical partition function and its relation to molecular partition function. The factorization of molecular partition function – translational, rotational, vibrational and electronic partition functions. Derivation of expressions for translational, rotational (diatomic) and vibrational partition functions. Relationship between partition functions and thermodynamic functions. The relationship between partition functions and thermodynamic functions. Law of equipartition energy.

Specific heats of solids – Einstein equation of heat capacity of solids – derivation. Explanation of heat capacity at very low and very high temperatures – Dulong and Petits Law. Debye theory.
The entropy of a monoatomic ideal gas. The Sackur-Tetrode equation- derivation. Mean translational and vibrational energies.

The relation between equilibrium constant and partition function- derivation.

Basic ideas of Bose-Einstein statistics and Fermi-Dirac statistics and comparison of these with Maxwell-Boltzmann statistics.

PC-18: Non-equilibrium Thermodynamics (15hrs)

Thermodynamic criteria for non-equilibrium states. Entropy production in irreversible processes. Entropy production in heat flow and entropy production in material flow.

Fluxes and forces. Linear flux-force relations**.** Phenomenonological equations and coefficients. Microscopic reversibility. Onsager reciprocal relations.

Application of Onsager relations to electrokinetic phenomena – electroosmotic pressure and streaming current. The Onsager relations and the principle of detailed balance. Liquid junction potentials – derivation of equation for liquid junction potential in terms of transport numbers using Onsager relations. Steady states. Principle of minimum entropy production.

Irreversible thermodynamics as applied to biological systems - examples.

Application to thermoelectric circuits. Seebeck and Peltier effect.

PC-19: Chemical kinetics – II: (15hrs)

Reactions in solution: Factors affecting reaction rates in solution. Effect of pressure on rate of reaction. Diffusion controlled reactions. Influence of dielectric constant and ionic strength on ion-ion, ion-dipole and dipole-dipole reactions. Primary and secondary salt effects. Kinetic isotope effects: Primary and secondary isotope effects. Solvent isotope effects.

Fast reactions: Flow methods and the stopped-flow technique. The fluorescence technique. Shock tube method. Relaxation methods (T-jump and P- jump). Kinetic equations for chemical relaxation.

Enzyme kinetics: Michaelis - Menten mechanisms of enzyme catalyzed reactions involving one and two intermediates. Steady-state approximation. Derivation of kinetic equations. Evaluation of kinetic parameters. Enzyme- substrate complex: Fischer's lock and key and Koshland's induced fit hypotheses. Specificity of enzyme-catalyzed reactions. Discussion of the various types of forces involved in the formation of E-S complex. pH dependence of enzyme-catalyzed reactions – the kinetics and the equations involved.

PC –20 : Electrochemistry – II (15 hrs)

The electrode-electrolyte interface: The electrical double layer. The Helmholtz-Perrin parallel-plate model, the Gouy-Chapman diffuse-charge model and the Stern model. Quantum aspects of charge transfer at the interfaces. Tunneling.

Electrodics: Charge transfer reactions at the electrode-electrolyte interface. Exchange current density and overpotential. Derivation of Butler-Volmer equation. High field approximation. Tafel equation - low field - equilibrium, Nernst equation. The symmetry factor and its significance.

Corrosion: Electrochemical corrosion.Short-circuited energy producing cell. The definition and final expression of corrosion current and corrosion potential. Homogeneous theory of corrosion.Evans diagrams. Potential-pH (Pourbaix) diagrams of iron. Methods of corrosion rate measurement. Mechanism of anodic dissolution of iron. Protection against corrosion. Corrosion inhibition by organic molecules.

Books suggested:

1. Elements of Statistical Thermodynamics, L. K. Nash, Addison – Wesley
2. Introduction to Statistical Thermodynamics, T. L. Hill, Addison Wiley
3. Statistical Thermodynamics, M. C. Gupta, New Age International
4. Atkin's Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press
5. Molecular Thermodynamics, D. A. McQuarrie & J. D. Simon, University Science Books
6. Text book of Biochemistry by Stryer, W.H.Freeman & Co Ltd
7. Advanced physical chemistry by Gurtu and Gurtu, Pragati Edition
8. Physical chemistry by Puri and Sharma, Vishal Publishing Co.
9. Chemical Kinetics, K. J. Laidler, McGraw Hill
10. Kinetics and Mechanism, A. A. Frost & R. G. Pearson, John Wiley & sons
11. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman & J. Kuriacose, McMillan
12. Chemical Kinetics and Reaction Mechanisms, J. H. Espenson, McGraw Hill
13. Physical Organic Chemistry, N. S. Isaacs, ELBS

14. The Physical basis of Organic Chemistry, Howard Maskill, Oxford University Press
15. Modern Electrochemistry, J. O. M. Bockris & A. K. N. Reddy, Plenum.
16. Modern Electrochemistry 2B, Bockris & Reddy, Plenum.
17. Introduction to Electrochemistry, S. Glasstone, EAST-WEST Press Pvt. Ltd, New Delhi

PAPER- CH(PC) 402T: SUPRAMOLECULAR CHEMISTRY, PHOTO CHEMISTRY AND COMPUTATIONAL CHEMISTRY

PC-21 : Supramolecular Chemistry
PC-22 : Photochemistry
PC-23 : Computational Chemistry
PC-24 : Theoretical treatment of bio polymers

PC-21: Supramolecular Chemistry

Concepts: Molecules, super molecules and supramolecules. Nature of Supramolecular interactions.

Molecular recognition – factors involved. Ionophores. Molecular receptors – design principles.

Molecular receptors for alkali metal ions, ammonium ions, anions and neutral molecules. Crown ethers, cryptands, spherands, calixaranes, and cyclodextrins - their selectivity, macrocyclic, and template effects. Fullerenes as supramolecules.

Threading of a linear molecule through a cyclic molecule –creation of Rotaxanes and Catenanes.

Thermodynamics of host-guest complexation. Enthalpy and entropy contributions. Complexation free energies.

Supramolecular catalysis- Crownether supported alkaline earth metal ions as catalysts, cyclodextrins and calixaranes as catalysts in chemical reactions. Transport of ions across membranes by biological molecules.

Molecular electronic devices: Molecular wires, molecular switches and machines.

PC-22: Photochemistry – Ii

Formation of excimers and exciplexes – PE diagram and quantum yields. Energy transfer mechanism for bimolecular quenching. Long-range coulombic energy transfer – critical transfer distance. Short-range electron exchange energy transfer. Triplet-triplet energy transfer and sensitization.

P-type delayed fluorescence. The experimental study of photochemical reactions: Product analysis, chemical methods in the study of intermediates, spectroscopic methods, ESR and CIDNP, rate coefficients for photochemical processes and identification of excited states.

Electronic transitions in transition metal complexes. Ligand field (LF) and charge transfer (CT) electronic states. $Ru(bpy)_3^{2+}$ as sensitizer for photoredox reactions, examples. Photochemical cleavage of water.

PC-23: Computational treatment of many electron systems (15hrs)

Multi-electron atoms. The antisymmetry principle and the Slater determinant. The Hartree-Fock method. The Hartree-Fock equations.(no derivation). The Fock operator. Core hamiltonian. Coulomb operator and exchange operator. Slater-type orbitals (STOs) as basis functions. Orbital energies and total energy. Helium atom example. Koopman's theorem. Hund's rules and theoretical basis of the Aufbau principle. Electron correlation energy.

The Hartree-Fock method for molecules. Restricted and unrestricted HF calculations. The Roothan equations. The Fock matrix. The Roothan matrix elements. GTOs and different types of basis sets. Minimal basis set. Model HF calculations on H_2. Discussion of results of HF calculations on simple molecules – H_2O and NH_3. Introduction to configuration interaction.

Density functional theory (DFT). Hohenberg-Kohn theorem. Kohn-Sham (KS) formulation of DFT. KS equations and KS orbitals. Brief explanation of exchange-correlation energy and exchange- correlation potential.

PC-24: Theoretical treatment of biopolymers (15 hrs)

Types of biopolymers. Methods of determining Size and shape of biopolymers - mean molecular masses, colligative properties, sedimentation, viscosity, light scattering methods.

Chain conformation and configuration of poly peptides. Random coils and measures of size – contour length, rms separation, radius of gyration, constrained chains.

Secondary structures of proteins- helices and sheets: The Corey-Pauling rules. Conformational energy of a polypeptide- bonding, nonbonding potentials, electrostatic interactions, dipole-dipole interactions and van der Waals interactions. Hydrogen bonds. Principles of molecular mechanics to calculate potential energy of a polypeptide. Ramachandran plots of α-helix and β-sheet.

Conformational entropy. Introductory treatment of the protein folding problem.

Books suggested:

1) J.W Steed and J.L Atwood, Supramolecular chemistry, John Wiley & Sons, Ltd. New York.
2) Piet W. N. M. van Leeuwen, Supramolecular Catalysis, Wiley-VCH Verlag GmbH & Co.
3) Principles and methods in supramolecular chemistry, Hans-Jorg Schneider and A.Yatsimirsky, John Wiley and Sons.
4) Analytical Chemistry of Macrocyclic and Supramolecular Compounds, S.M.Khopkar, Narosa Publishing House
5) Essentials of Molecular Photochemistry, A. Gilbert & J. Baggott, Blackwell Science
6) Quantum Chemistry, I. N. Levine, Prentice Hall
7) Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedman, Oxford University Press
8) Introduction to Computational Chemistry, F. Jensen, John Wiley & Sons
9) Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill
10) Modern Quantum Chemistry, A. Szabo and N. S. Ostlund, Dover publishers
11) Computational Chemistry: Introduction to the theory and Applications of Molecular and Quantum Mechanics, Errol Lewars, Springer Publications
12) Physical Chemistry, D. A. McQuarrie and J. D. Simon, Viva Books Ltd.
13) Physical Chemistry, P. W. Atkins, Oxford Unibersity Press.

14) Approximate Molecular Orbital Theory, J. A. Pople and D. L. Beveridge, McGraw Hill
15) Biophysical Chemistry, Cantor & Schimmel, W. H. Freeman and Company
16) Principles of Physical Biochemistry, Kensal E van Holde, W. Curtis Johnson & P. Shing Ho, Prentice Hall
17) Physical Biochemistry : Principles and Applications, David Sheehan, John Wiley
18) Physical Chemistry for the Chemical and Biological Sciences, Raymond Chang, University Science Books

ELECTIVE –3A:

PAPER III CH(PC)- 403T(CB1): CATALYSIS

PC(CB1)-17: Homogeneous catalysis
PC(CB1)-18: Surface Chemistry & Micellar catalysis
PC(CB1)-19: Heterogeneous catalysis
PC(CB1)-20: Phase transfer , Anchored & Photo catalysis

PC(CB1)-17: Homogeneous catalysis (15 hrs)

Introduction to catalysis. Types of catalysis, characteristics of catalyst, catalyst supports, promoters, general mechanism of catalysis, equilibrium treatment and steady state treatment. Activation energies of catalyzed reactions.

Acid-base catalysis, specific acid-base catalysis, general acid base catalysis, mechanism of acid – base catalysis, catalytic activity and acid-base strength- Bronsted relationships.
Acidity functions: Types of acidity functions. Hammett acidity function. Measurement of Hammett acidity function(Ho), usefulness of Hammett acidity function in understanding the mechanism of an acid catalyzed reactions. Zucker-Hammett hypothesis and its applications. Bunnett – Olson's criteria of acid-base catalyzed reactions with examples.

Catalysis by transition metal ions and their complexes. Use of Ziegler –Natta and metallocene catalysts as homogeneous catalysts for polymerization of olefins. Application of metal ion catalysis to the hydrogenation of alkenes, hydroformylation, oxidation and isomerization reactions. Asymmetric Catalysis–Introduction, Catalysts, Commercial Applications, Asymmetric Hydrogenation, Enantioselective Isomerization: L-Menthol, Asymmetric Epoxidation.

PC(CB1)-18: Surface Chemistry and Micellar catalysis (15hrs)

Surface tension. Curved interfaces. The Laplace equation. Capillary action. Thermodynamics of surface layers – Gibbs isotherm.

Adsorption. Types of adsorption, factors effecting adsorption, Chemistry and thermodynamics of adsorption. Determination of heats and entropies of adsorption.

Surface versus bulk structures. Adsorbate -induced restructuring of surfaces. Thermal activation of bond breaking on a surface. Co-adsorption. Chemisorption isotherms. Kinetics of chemisorption.

Surface films. Monometallic surfaces and bimetallic surfaces. Experimental techniques for the study of monolayer films. States and reaction in monomolecular films. Reaction between $H_2(g)$ and $N_2(g)$ catalyzed by surfaces to give $NH_3(g)$.

Micelles: Classification of surface active agents. Micellization and micellar interactions. Structure of micelles – spherical and laminar. Critical micellar concentration (CMC). Factors affecting the CMC of surfactants.

Counter ion binding to micelles. Thermodynamics of micellization. Phase separation and mass action models, solubilization, micro emulsion, reverse micelles. Reactions assisted by micelle formation. Examples of micelle-catalyzed reactions and their mechanisms.

PC(CB1)-19: Heterogeneous catalysis (15 hrs)

Heterogeneous catalysis. Broad categories of catalysts – metals, bimetals, semiconductors, insulators, zeolites, oxides, nano materials.

Preparation of metal catalysts, supported metal catalysts and non- metallic catalysts. Co-precipitation, Impregnation, sol-gel method, deposition-precipitation, hydrothermal synthesis, pulsed laser methods, plasma chemical methods, chemical vapor deposition methods

Steps in heterogeneous catalyzed reactions. Diffusion and adsorption. Mechanism of surface-catalyzed reactions. Adsorption isotherms - Langmiur Hinshelwood model, Rideal - Eley mechanism, Kinetics and thermodynamics of catalysed reactions. Catalytic activity – the determining factors. Structure sensitive and structure insensitive catalysts.

Characterization of catalysts: Surface area by BET method. Determination of pore volume and pore size distribution by BJH method. Pore size and specificity of catalysts. Surface acidity of catalysts- Determination of surface acidity by indicator method, IR spectroscopic method and TPD methods. Surface characterization by XRD, LEED, TEM & AFM, XPS, AES, techniques.

Auto exhaust emissions- catalytic converters. Catalytic hydrogenation and oxidation reactions.

Cracking and reforming. Fischer-Tropsch synthesis of methanol.

PC(CB1)-20: Phase transfer, Anchored and Photo catalysis **(**15 hrs)

Phase-transfer catalysis (PTC): Principles of phase-transfer catalysis. PTC classification.
Role of water in phase-transfer catalyzed reactions. Factors influencing the rate of PTC reactions.

Inverse phase transfer catalysis. Mechanism of nucleophilic displacement reactions.

Crown ethers: Crown ethers as phase transfer catalysts(PTC) in the reaction of alkyl halides with super oxide. Permanganate oxidation of alkenes and phenols in presence of PTC's viz., quarternary ammonium salts and crown ethers.

Anchored catalysis: Definition and examples of anchored catalysis- organic polymers, inorganic oxides and clays as supports. Structure of montmorillonite anchored catalysts- HEW structure and EF structure. Montmorillonite anchored catalysts- application of intercalated clay catalysts in hydrogenation reactions.

Photo catalysis: Photocatalytic effect, metal semiconductor systems as photo catalysts, nature of the metal loaded, extent of metal loading, nature of semiconductor, doped semiconductors, coupled Semiconductors. Application of photocatalysis for splitting of water by semiconductor particles, removal of organic and inorganic pollutants, for oxidation and reduction of organic compounds.

Books suggested:

1. Principles of Heterogeneous Catalysis in practice, G. C. Bond, Oxford Publishing
2. Heterogeneous Catalysis, C. Satterfield, McGraw Hill
3. Catalysis, Principles and applications, edited by B. Vishwanathan, S. Sivasanker & A. V. Rama Swamy, Narosa Publishing House
4. Catalysis, J. C. Kuriacose, Macmillan
5. Colloidal and surface chemistry , M. Satake, Y. Hayashi, Y.Mido, S.A.Iqbal and M.S.sethi
6. " Physical Organic Chemistry" by L.P.Hammett, chapter 9 , McGraw Hill .
7. Chemical Review, **57,** 1935(1957), M.A. Paul and F.A. Long
8. Phase Transfer Catalysis, Fundamentals, Applications and Industrial perspective, C. M. Stark, C. Liotta & M. Halpern, Academic Press
9. Phase Transfer Catalysis, E. V. Dehmlow & S. S. Dehmlow, Verlag Chemie, Weinheim
10. Phase Transfer Catalysis in Organic synthesis, W. P. Weber & G. W. Gokel, Springer
11. Hand book of phase transfer catalysisEdited by Y. Sasson and R. Neumann
12. Catalysis in Micellar and Macromolecular systems, J. H. Feudler & E. J. Feudler, Acad. Press
13. Reaction Kinetics in Micelles, E. H. Codes (ed), Plenum
14. Micelles – Theoretical and Applied aspets, V.Moroi, plenum
15. Physical Chemistry of surfaces, A.W.Adamson and A.P.gast, Wiley
16. Polymer supported Catalysts, C. U. Pittman Jr, vol 8, Comprensive Organometallic Chemistry
17. Principles and Practice of Heterogeneous Catalysis, J. M.Thomas andW.J.Thomas, VCH1997.
18. Spectroscopy in catalysis – An introduction by J. W. Niemantsverdriet.
19. Modern methods of Organic Synthesis: Ahluwalia.

ELECTIVE–3B

PAPER IV CH(PC) 403 T(CB2) : Dynamics of Chemical Reactions And Sensors

PC-(CB2)-21: MO and VB theory of reactivity
PC-(CB2)-22: Kinetic, isotopic, structural, solvent, steric and conformatlonal effects
PC-(CB2)-23:Nucleophilic, electrophilic and free radical reactivity
PC-(CB2)-24: Sensors

PC-(CB2)-21: Molecular Orbital (MO) and Valence Bond (VB) theory of reactivity 15 Hrs

Introduction to Huckel molecular orbital (MO) method as a means to explain modern theoretical methods. Advanced techniques in PMO and FMO theory. Molecular mechanics, semiemperical methods and ab inito and density functional methods. Scope and limitations of several computational programmes. Quantitative MO theory-Huckel molecular orbital (HMO) method as applied to ethane energy levels .Orbital symmetry, orbital interaction diagrams. MO of simple organic systems such as ethane, allyl, butadiene, methane and methyl group. Conjugation and hyperconjugation. Aromaticity. Valence bond (VB) configuration mixing diagrams. Relationship between VB configuration mixing and resonance theory. Reaction profiles. Potential energy diagrams. Curve crossing model nature of activation barrier in chemical reactions. Principle of reactivity Mechanistic significance of entropy, enthalpy and Gibbs free energy. Arrhenius equation, transition state theory. Uses of activation parameters.

PC-(CB2)-22: Kinetic, isotopic, structural, solvent, steric and conformational effects 15 Hrs

Theory of isotope effects, Primary and secondary kinetic isotope effects. Heavy isotope effects. Tunneling effect Solvent effects. Structural effects on reactivity: Linear free energy relationship (LFER.). The Hammett equation, substituent constants, theories of substituent effects. interpretation of σ-values. Reaction constant ρ. Deviations from Hammett equation. Dual—parameter correlations, inductive substituent constant The Taft model, σ1, σR scales. Solvation and solvent effects: Qualitative understanding of solvent- solute effects on reactivity Thermodynamic measure of solvation. Effects of solvation on reaction and equilibrium. Various empirical indexes of solvation based on physical properties, solvent- sensitive reaction rates, spectroscopic properties and scales for specific solvation. Use of solvation scales in mechanistic studies. Solvent effects from the curve-crossing model. Various type of steric strain and their influence on reactivity. Steric acceleration. Molecular measurements of steric effects upon rates. Steric LFER. Conformational barrier to bond rotation-spectroscopic detection of individual conformers. Acyclic and monocyclic systems. Rotation around partial double bonds. Winstein-Holness and Curtin-Hammet principle.

PC-(CB2)-23: NUCLEOPHILIC, ELECTROPHILIC AND FREE RADICAL REACTIVITY 15 Hrs

Bases, nucleophiles, Electrophiles and Catalysts. Acid-base dissociation. Electronic and structural effects, acidity and basicity. Acidity functions and their applications. Hard and soft acids and bases. Nuccleophilicity scales, Nucleofugacity. The α-effect.- Ambivalent nucleophiles. Acid-base catalysis. Specific and general catalysis. Bronstéd catalysis. .nucleophilic and electrophilic catalysis. Catalysis by non-covalent binding micellar catalysts. Nucleophilic and electrophilic Reactivity:Structural and electronic effects on SN1 and SN2 reactivity. Solvent effects,kinetic isotope effects. Intramolecular assistance. Electron transfer nature of SN2 reaction. Nuclcophilicity and S2 reactivity based on curve-crossing rnodel. Relationship between polar and electron transfer reactions. SRN1 mechanism. Electrophilic reactivity, general mechanism. Kinetics of SE2-Ar reaction, Structural effects on rates and selectivity. Curve crossing approach to electrophilic reactivity. ; Radical and pericyclic reactivity. (a)Radical stability, polar influences, solvent and steric effects. A curve crossing approach to radical addition, factors affecting barrier heights in additions, regioselectivity in radical reactions. Reactivity, specificity and periselectivity in pericyclic reactions.

PC-(CB2)-24: Chemical, Electrochemical and Bio Sensors 15hrs

Importance of Sensors, Biomolecular recognition elements, Artificial molecular-recognition materials, Molecular imprinted polymers, Electrode modification. Fluorescence, chemi and bio-luminescence sensors, Fluorescent tag molecules, Applications. Conductometric sensors, Coulometric sensors, Voltammetric sensors, Applications, Neurotransmitters, Amperometric sensors, Chronoamperometric analysis, Multichannel sensors, Microelectrode sensors, Electrochemical Impedance Sensors, Quartz crystal nanobalance sensors, Molecular recognition, Applications. Surface Plasmon resonance based sensors, Fiber optic sensors, Twodimensional microarray based sensors, Applications for Food Safety - Mycotoxins, adultrants, Biomedical diagnosis - Cancer markers.

Books suggested:

1. Molecular mechanics. By U.Bukert and N.L.Allinger, ACS Monograph 177,1982
2. Organic Chemistry book of Orbitals. L.Salem and W.L.Jorgenson
3. Mechanism and theory in Organic Chemistry, T.M.Lowry, K.C.Richardson, Harper and Row
4. Introduction to theoretical Organic Chemistry and molecular modeling by W.B.Smith, VCH, Weinhein.
5. Physical Organic chemistry, N.S.Isaaçs
6. Suprarnolecular Chemistry - concepts and perspectives by J M .Lehn,
7. The Physical basis of Organic Chemistry by H.Maskill.
8. Physical Organic Chemistry by Jack HineLaboratory course
9. Brian R. Eggins, Chemical Sensors and Biosensors, Analytical Techniques in the Sciences (ANTS), 2nd Edition, Wiley, 2002.
10. Gabor Harsanyi, Sensors in Biomedical Applications - Fundamentals, Technology and Applications, CRC Press, 2000.
11. Raluca-Ioana Stefan, Electrochemical Sensors in Bioanalysis, CRC Press, 2001.

ELECTIVE –4A (ID PAPER)

PAPER III CH(PC)- 403T(CB3): MOLECULAR MODELING AND IT'S APPLICATIONS

PC(CB3)-25: Molecular Modeling – I
PC(CB3)-26: Molecular Modeling – II
PC(CB3)-27: Drug Design Methods I - Ligand Based
PC(CB3)-28: Drug Design Methods II - Structure Based.

PC(CB3)-25: Molecular Modeling – I (15hrs)

Introduction to Molecular Modeling, Single molecule calculations, assemblies of molecules and reactions of molecules - Co-ordinate systems: Cartesian and Internal Co-ordinates, Z-matrix - Potential energy surface - Conformational search; Global minimum, Local minimum, Conformational analysis of ethane.

Force field ; Features of Molecular Mechanics, Bonded and Non-bonded interactions, Bond Stretching, Angle Bending, Torsional Terms (Improper Torsions, out of Plane Bending Motions, Cross Terms), Non Bonded Interactions (Electrostatic Interactions, Van-der Waals interactions), Hydrogen Bonding Interactions.

PC(CB3)-26: Molecular Modeling – II (15hrs)

Force Field Equation in Energy minimization (Energy as function of r, θ, ω) - Introduction to Derivative Minimization Methods (First Order Minimization), Types of energy minimization Methods ; Steepest Descent, Conjugate Gradient, Conformational Search procedures - Geometry optimization procedures - Molecular Dynamics: Introduction, description of Molecular Dynamics, basic elements of Monte-Carlo method, differences between Molecular Dynamics and Monte-Carlo method, Qualitative exposure to Molecular Dynamics Simulations.

PC(CB3)-27: Drug Design Methods I - Ligand Based (15hrs)

Lead Molecule - Structure Activity Relationship (SAR), Quantitative Structure Activity Relationship (QSAR), Distinguish between SAR and QSAR - Physicochemical parameters ; Electronic effects, Hydrophobicity, Steric Factors Taft's Steric function, Molar Refractivity, Verloop Steric factor - Molecular Descriptor analysis: Craig plot, Topliss scheme, Bioisosteres - Hansch model, Free-Wilson model for QSAR equations - Regression analysis: Multi Linear Regression and Partial Least Square (terms: n, SD, r, r^2, r^2%, F) - Examples for linear and non-linear equations - 3D QSAR: CoMFA and CoMSIA - Differences between 2D and 3D QSAR.

PC(CB3)-28: Drug Design Methods II - Structure Based. (15hrs)

Database similarity searches - Pair-wise alignment: Global sequence analysis (Needleman-Wunsch), Local Sequence Alignment (Smith Waterman), Multiple Sequence Alignment - Homology Modeling: Query sequence, Template selection, Alignment, Backbone Modeling, Loop Modeling, Side chain Modeling, Model optimization, Energy minimization - Model Evaluation: Ramachandran Plot, Verify 3D, Errata and ProSA - Active site Identification - Docking, Docking Algorithms: Genetic Algorithm, Incremental construction - Molecular Interactions, Scoring functions - Virtual Screening: Ligand Based and Structure Based. De novo ligand design and its limitations.

Books suggested:

1. Molecular Modelling: Principles and Applications, by Andrew Leach, Longman Publications.
2. Computational Chemistry, Guy H. Grant & W. Graham Richards, Oxford University Press.
3. Computational Chemistry: Introduction to the theory and Applications of Molecular and Quantum Mechanics, Errol Lewars, Springer Publications.
4. Recent advances in Bioinformatics by I. A. Khan and A Khanum Ukaaz publications, 2003.
5. Molecular modelling – Basic Principles and Applications by Hans Dieter Holtje and Gerd Folkers, Wiley-VCH, 1996
6. Introduction to Computational Chemistry by Jensen, Wiley Publishers, second edition
7. Bioinformatics – A Primer by P. Narayanan, New Age International, (PC) Ltd, 2005.
8. Introduction to Bioinformatics by Arthur M. Lesk, Oxford University Press (Indian. Edition), 2002
9. Principles of Medicinal Chemistry Vol. II by Dr. SS Kadam Pragati books Pvt. Ltd; 2007
10. An Introduction to Medicinal Chemistry by G L Patrick, Oxford University Press
11. Bioinformatics: Methods and Applications: Genomics, Proteomics and Drug Discovery. S.C. Rastog, Namita Mendiratta, Parag Rastogi, PHI Larning Pvt. Ltd; 2006
12. Pharmacy Practice Vol.I and II by Remington, Pharmaceutical Press
13. Burger's Medicinal Chemistry and Drug Discovery, 5th Edition, Wiley-Interscience, New York
14. Text book of Drug design and Vol.1 discovery 3rd Edition by POVL krogsgaard- Larsen Tommy liljefors and ULF Madsen.

ELECTIVE –4B (ID PAPER)

PAPER-IV CH(PC) 404T(CB4): Engineering Chemistry

PC(CB4) -29: Water And Waste Water Treatment
PC(CB4) -30: Corrosion And Its Control
PC(CB4) -31: Energy Sources
PC(CB4)- 32 Engineering Materials

PC(CB4) -29:Water and waste water treatment (15 hrs)

Review of Hardness: causes, measurement of hardness, units- types of hardness, estimation of temporary and permanent hardness, numerical problems. Boiler troubles- scales and sludge formation, caustic embrittlement, priming and foaming. Methods for boiler water treatment: Soda-lime process, zeolite process, ion exchange process. Treating saline water: distillation, electrodialysis, reverse osmosis. Municipal water supply: sedimentation, filtration, sterilization. Waste water treatment: physical, chemical and biological treatment. Sewage water , COD and BOD , numerical problems

PC(CB4) -30:Corrosion and its control: (15 hrs)

Magnitude of the problem, theories of corrosion, Chemical and electrochemical corrosion, corrosion reactions, factors affecting corrosion- nature of metal, purity of metal,electrochemical series, over voltage, nature of oxide film, nature of corrosion product, nature of environment, effect of temperature, effect of pH, effect of oxidant, humidity. Corrosion control methods-design and material selection, cathodic protection, sacrificial anode, impressed current cathode. Surface coating methods: Surface preparation, metallic coatings, application of metal coatings: hot dipping, galvanizing, tinning, cladding, electroplating, chemical conversion coatings. Organic surface coatings-paints, constituents of paints and their functions, methods of application of paints, failure of paint films, varnishes, enamels, lacquers.

PC(CB4) -31: Energy sources: (15 hrs)

Conventional energy resources: Chemical fuels, classification, (solids, liquids, gaseous) . Solid fuels: coal, analysis of coal , proximate and ultimate analysis and their significance. Liquid fuels: petroleum, refining of petroleum, cracking, reforming. Synthetic petrol - Bergius and Fischer-Tropsch's process, knocking, anti knocking agents, octane number. Diesel fuel: Cetane number. Other liquid fuels: LPG, biodiesel, kerosene, fuel oil, benzol, tar, power alcohol. Gaseous fuels: natural gas, coal gas, producer gas, oil gas, water gas, biogas, Combustion: Calorific value and its determination, bomb calorimeter. HCV and LCV values of fuels, problems. analysis of flue gas by Orsats method. Rocket fuels, solid propellants, liquid propellants, monopropellants, bipropellants.

Non conventional energy resources: Nuclear fuels- nuclear reactor, nuclear fission, nuclear fusion, sources of nuclear fuels, disposal of radio active wastes, reprocessing of nuclear fuels. solar, hydro, wind, tidal energies. Bio fuels, H_2 as a non polluting fuel.

PC(CB4) -32: Engineering materials. (15 hrs)

Cement: composition of Portland cement, analysis, setting and hardening of Portland cement (reactions), decay of cement concrete, lime, manufacture, types of lime, plaster of paris

Lubricants: Criterion of a good lubricant, classification of lubricants: petroleum oils, fixed oils, synthetic lubricants, semisolid lubricants, solid lubricants. Properties of lubricants: cloud point, pour point, flash and fire point, viscocity.

Refractories: Classification, characteristics of good refractory, failure of refractories. Glass, glass making oxides and their functions, manufacture of glass. Porcelain, enamels, abrasives.

Conductors and insulators: Classification of insulators, characteristics of thermal and electrical insulators and super conductors (Nb-Sn alloy, $YBa_2Cu_3O_{7-x}$) applications.

Composite materials: Advantageous properties of the composites, classification, mechanism of strengthening, mechanism of hardening of particle reinforcement, fabrication of the composites.

Liquid crystals: Characteristics of liquid crystal orders, physical properties of liquid crystals, classification of Liquid crystals, types of mesophases chemical nature of Liquid crystals, applications of Liquid crystals, future of liquid crystals.

Books suggested:

1.Text book of Engineering Chemistry by C.P. Murthy, C.V. Agarwal & A. Naidu: B.S. Publications, Hyderabad (2006).
2.Text book of Engineering Chemistry by S.S. Dara: S. Chand & Co. New Delhi (2006).
3.Engineering Chemistry by B. Siva Shanker : Mc-Graw Hill publishing Company Limited, New Delhi (2006)
4.Engineering Chemistry by J.C. Kuriocose &J. Rajaram,Tata McGraw Hill Co. NewDelhi (2004)
5.Engineering Chemistry by P.C. Jain & Monica Jain, Dhanpatrai publishing company, (2008)
6.Chemistry of Engineering Materials by C.V. Agarwal, C.P. Murthy & A. Naidu: BS publications
7.Chemistry of Engineering Materials by R.P. Mani & K.N. Mishra, CENGAGE learning
8.Applied Chemistry – A text book of engineering and Technology – Springar (2005)
9.Text book of Engineering Chemistry by Shasi Chawla: Dhanpatrai Publishing company, New Delhi (2008)
10. Engineering Chemistry by R. Gopalan, D. Venkatappayya & D.V. Sulochana Nagarajan – Vikas Publishers (2008).

ELECTIVE–4C (ID PAPER)

PAPER-IV CH(PC) 404T(CB5): Sugar Chemistry AND Sugar Technology

PC(CB5) -33: Advanced Sugar Chemistry
PC(CB5) -34: Sugar & Sugar byproducts
PC(CB5) -35: Methodology used in Sugar Analysis
PC(CB5)- 36: Sugar Technology and Management

PC(CB5) -33: Advanced Sugar Chemistry: (15 hrs)

Carbohydrate nomenclature. Fischer, Haworth and conformational structures of mono and oligo saccharides. Chemical reactivity of sugars. Reducing and non-reducing sugars. Chiral nature of sugars. R-S nomenclature, Fischer D-L nomenclature of sugars. Sugar enantiomers, diastereo isomers, epimers and enomers. Acyclic structure of sugars, determination of relative and absolute configuration of sugars. Cyclic forms of sugars. Conformational analysis of sugars. Hassel- Otter effect. Delta-two effect. Anomeric effect. Calculation of conformational free energies. Optical rotation, specific rotation and molecular rotation of sugars. General epimer rule. Relationship between rotation and conformation. Stereo chemical transformations. Mutarotation, enolization, isomerization, anhydride formation and reversion, pH stability of glucose and fructose, protection of sugar hydroxyls.

PC(CB5) -34: Sugar & Sugar byproducts: (15 hrs)

Structure determination of sucrose, synthesis of sucrose, biosynthesis of sucrose, chemical nature of sucrose. Oligo saccharide synthesis. Oligo saccharide optical rotating power (Hudson and Klyn rules). ^{13}C NMR spectroscopic data of glucose, fructose and sucrose. Uses of sugar chirons in organic synthesis. Sugar byproducts. Bagasse, molasses and press mud. Bagasse- characteristics and uses. Production of biogas, fiberboard and furfural. Press mud- extraction of cane wax, press mud and manure. Molasses- fermentation of molasses. Production of alcohol and rectified spirit.

PC(CB5) -35:Methodology used in Sugar Analysis: (15 hrs)

Sampling techniques. Determination of moisture in bagasse, molasses and cane sugar. Methods of estimation of total soluble solids in sugar and sugar house products. Optical methods of sugar analysis, sugar scales and normal weight. Estimation of reducing sugars and sugar present in cane juice by Eynon & Lane, Luff & Schoorl and Benedicts methods. Determination of sugars by Invertase method, Jackson- Gellis, Munsen- Walker's Cu_2O and De Whalleys' volumetric method. Determination of Ash by Carbonate- Ash and Cuitometeric (Conductometric) methods. Determination of various other constituents present in raw sugars. Estimation and chemical composition of cane and its juice.
Instrumental methods of sugar industry- Static characteristics and Dynamic characteristics. Gas, liquid, vapor thermometers. Bimetallic thermometers and thermocouples. Electronic panometer, cuitometer. Introduction to pneumatic control systems and elements. Working principle and instrumentation methodology of potentiometer, pH meter, polarimeter and cuitometer.

PC(CB5) -36: Sugar Technology and Basic Principles of Management: (15 hrs)
Sugar Technology: Cane juice interaction, maceration and imbibition. Principles of cane juice clarification, defecation and sulphitation. Juice heaters, filters and reaprovation vaccum pans. Centrifuges. Sugar driers and molasses. Introductory treatment of chemical control (i) Milling Control and (ii) Boiling house control.

Management: Concept and philosophy of management in major and small-scale industries. Location of factory site and Lay out of plant. Joint stock companies. Co-operative Societies. Production management and control. Personnel administration, purchases and sales, organization and control.

Books suggested:

1. Cane Sugar Hand Book, Maede & Chen, John Wiely & Sons
2. Determination of Food Carbohydrates, D. A. T. Southgate, Applied Science Publishers, London
3. Text Book of Sugar Chemistry and Sugar Technology, Mathur
4. Text Book of Sugar Byproducts, Morris Patrov
5. A Hand Book of Qualitative and Quantitative Organic Analysis, H. J. Clark, Orient Longman
6. Text Book of Biochemistry, Lehninger
7. Analysis of Sugars, Pleus
8. Text Book of Sugar Technology, Hugot
9. Instrumental Methods in Sugar Industry, Eckman
10. Principles of Instrumental Analysis, Skoog and West
11. Technical Methods of Analysis, Griffith, McGraw Hill
12. Advanced Sugar Chemistry, R. S. Shellaxberges
13. Sugar, John Yulkin, Jack Edelman, Liesel Hough
14. International Uniform Methods for Sugar Analysis, H. C. S. De Whelly

IV SEMESTER PRACTICALS

Note: The data obtained in all the experiments are to be analyzed by the students both *by the usual graphical methods and by regression (linear/nonlinear) techniques using a PC.*

CH (PC) 451P: Paper-V (Chemical Kinetics) 9hrs/week

- **Study of acetone-iodine reaction by spectrophotometry**
  1. Order w.r.t.[iodine]
  2. Order w.r.t. [acetone]
  3. Order w.r.t. [H^+]

- **Study of peroxydisulphate – iodide reaction by colorimetry**

- **Study of saponification of ethyl acetate by conductometry:**
  1. Overall order of the reaction
  2. Order w.r.t. [ethyl acetate]
  3. Order w.r.t. [NaOH]

♦ **Study of solvolysis of t-butylchloride by conductometry**:
effect of solvent dielectric constant/
polarizability (methanol/water mixture) on the rate of solvolysis

♦ **Study of oxidation of primary alcohols by dichromate by spectrophotometry**:
Application of Taft equation

CH (PC) 452P: Paper-VI (Instrumentation) 9 hrs/week

Spectrophotometry:

- Estimation of Cu(II) using EDTA
- Estimation of Fe(III) using thiocyanate
- Estimation of Fe(II) using 1,10-phenanthroline
- Estimation of Fe(III) in tap water using thiocyanate by standard addition method
- Simultaneous determination of dichromate and permanganate in a mixture
- Spectrophotmetric titrations: Cu(II) vs EDTA
  Fe(II) vs 1,10-phenanthroline
- Composition of Cu(II) – EDTA complex by Job's method
- Composition of Fe(II) – phenanthroline complex –Job's method, mole ratio, slope ratio method.
- Determination of composition and Gibbs energy of formation of Fe(III)–salicylic acid complex
- Determination of pK_a of methyl red indicator
- Estimation of Mn(II) by spetrophotometry using periodate.

Potentiometry:

- Potentiometric titrations:

1. Weak acids vs strong base and calculation of dissociation constants
2. Mixture of strong and weak acids vs strong base
3. Dibasic acid vs strong base
4. Fe(II) vs Ce(IV) and calculation of formal redox potential of Fe(II)/Fe(III)
   - Fe(II) vs MnO_4^-
   - Fe(III) vs EDTA
   - Mixture of halides vs $AgNO_3$
   - Mixture of KI and KSCN vs $AgNO_3$

Polarography:

- Estimation of Pb^{2+}, Cd^{2+} and Ni^{2+} separately and in a mixture.

Suggested books:

1. A textbook of practical organic chemistry by A I Vogel, Vol 1&2.
2. Senior practical physical chemistry. B. D. Khosla, V.C. Garg, Adarsh Gulati
3. Experimental Physical Chemistry: V. Athawale and P. Mathur.
4. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.
5. Practical in Physical Chemistry: P.S. Sindhu
6. Advanced Practical Physical chemistry: J.B.Yadav