

**Proposed Syllabus
for
M.Sc. Chemistry
(NEP)**

CHOICE BASED CREDIT SYSTEM



**Department of Chemistry
CSJM UNIVERSITY, CAMPUS
Kanpur**

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CHHATRAPATI SHAHU JI MAHARAJ UNIVERSITY, KANPUR

STRUCTURE OF SYLLABUS FOR THE

PROGRAM: M.Sc., SUBJECT: Chemistry (University Campus)

1 ST YEAR / 1 ST SEM						
COURSE CODE	TYPE	COURSE TITLE	MIN CREDITS	CIA	ESE	MAX. MARKS
B02U0701T	CORE	Inorganic Chemistry I	4	25	75	100
B02U0702T	CORE	Organic Chemistry I	4	25	75	100
B02U0703T	CORE	Physical Chemistry I	4	25	75	100
B02U0704T	CORE	Analytical Chemistry	4	25	75	100
B02U0705P	PRACTICAL	Inorganic chemistry Practical	4	25	75	100
	PROJECT	RESEARCH PROJECT				-
TOTAL			20			500
1 ST YEAR / II ND SEM						
B02U0801T	CORE	Inorganic Chemistry II	4	25	75	100
B02U0802T	CORE	Organic Chemistry II	4	25	75	100
B02U0803T	CORE	Physical Chemistry II	4	25	75	100
B02U0804T	ELECTIVES	1. Environmental Chemistry	4	25	75	100
B02U0805T		2. Liquid State				
B02U0806P	PRACTICAL	Organic Chemistry Practical	4	25	75	100
B02U0807R	PROJECT	RESEARCH PROJECT	8	25	75	100
MINOR ELECTIVE FROM OTHER FACULTY (IN 1 ST YR- Ist/II nd SEM)*			4/5/6	25	75	100
TOTAL			32			700
II ND YEAR / III RD SEM						
B02U0901T	CORE	Applications of Spectroscopy	4	25	75	100
B02U0902T	CORE	Advance Principles of Physical Chemistry	4	25	75	100
B02U0903T	ANY TWO ELECTIVES TO BE CHOSEN	1. Bioinorganic, Nuclear and Supramolecular Chemistry	4	25	75	100
B02U0904T		2. Bio-organic Chemistry				
B02U0905T		3. Nano Chemistry				
B02U0906T	CHOSEN	4. Pharmaceutical Chemistry	4	25	75	100
B02U0907P	PRACTICAL	Physical Chemistry Practical	4	25	75	100
	PROJECT	RESEARCH PROJECT				-
TOTAL			20			500
II ND YEAR / IV TH SEM						
B02U1001T	ANY THREE ELECTIVES TO BE CHOSEN	Advanced Organic Chemistry	5	25	75	100
B02U1002T		Advanced Physical Chemistry				
B02U1003T		Advanced Inorganic Chemistry				
B02U1004T		Applications of Chemistry in Industries				
B02U1005T		Physical Methods in Chemistry				
B02U1006T		Green Chemistry				
B02U1007T		Photochemistry				
B02U1008T		Materials Chemistry				
B02U1009T		Chemistry of Materials, Petrochemicals and Fertilizers				
B02U1010T		Waste Management				
B02U1011T	CORE	Polymer Chemistry	5	25	75	100
B02U1012R	PROJECT	RESEARCH PROJECT	8	25	75	100
TOTAL			28			500
GRAND TOTAL			100			2200

NOTE:

Rohini *Ratna*

NOTE:

1. *A MINOR ELECTIVE FROM OTHER FACULTY SHALL BE CHOSEN IN 1ST YEAR (EITHER Ist / IInd SEMESTER) AS PER AVAILABILITY.
2. In both years of PG program, there will be a Research Project or equivalently a research-oriented Dissertation as per guidelines issued earlier and will be of 4 credit (4 hr/week), in each semester. The student shall submit a report/dissertation for evaluation at the end of the year, which will be therefore of 8 credits and 100 marks
3. Research project can be done in form of Internship/Survey/Field work/Research project/ Industrial training, and a report/dissertation shall be submitted that shall be evaluated via seminar/presentation and viva voce.
4. The student straight away will be awarded 25 marks if he publishes a research paper on the topic of Research Project or Dissertation.

Semester I

Inorganic Chemistry-I Paper Code: B02U0701T

Credits: 4

Unit 1: Chemical Bonding

Walsh diagram; Evidence of MO pictures from spectra and reactivity; Molecular term symbols (ground & excited state). $p\pi - d\pi$ bonding, $3C-2e$ bonding, μ -bond, δ -bond.

Unit 2: Coordination Chemistry

Crystal field theory, Splitting of d orbitals. Crystal field stabilization energies in weak field and strong field environments, spectrochemical series. and Jahn-Teller effects on energy levels.

Unit 3: Magnetochemistry

Van Vleck equation and its applications, Curie and Curie-Weiss laws, zero-field splitting, spin-orbit coupling, quenching of orbital contribution, para and diamagnetism, ferromagnetic, ferrimagnetism & antiferromagnetic coupling.

Unit 4: Metal Ligand Equilibrium

Equilibria Stability of mononuclear, polynuclear mixed ligand complexes in solution, Stepwise and overall formation constants, trends in stepwise constants factors affecting the stability of metal complexes – chelate effect, determination of stability constants

Unit 5: Reaction Mechanism

Inert and labile complexes-Explanation of lability on the basis of CFSE. Substitution reactions (dissociative, associative, Id, & Ia mechanisms) in square planar, tetrahedral and octahedral geometries with special reference to d^n ion complexes.

Books Recommended:

1. D. F. Shriver, P. W. Atkins and C. H. Langford, *Inorganic Chemistry*, Oxford University Press, New York (1990.)
2. B. Douglas, D. McDaniel and J. Alexander, *Concepts and Models of Inorganic Chemistry*, 3rd Edn, John Wiley and Sons, Inc., New York (2001).
3. J. E. Huheey, E. A. Keiter and R. L. Keiter, *Inorganic Chemistry: Principles of Structure and Reactivity*, 4th Edn, Harper Collins College Publishers, New York (1993).
4. T. P. Fehlner, J. -F. Halet and J. -Y. Saillard, *Molecular Clusters — A Bridge to Solid State Chemistry*, Cambridge University Press, Cambridge (2007).
5. M. Driess and H. Noth (Eds.), *Molecular Clusters of the Main Group Elements*, Wiley-VCH, Weinheim (2004).
6. O. Kahn, *Molecular Magnetism*, VCH, New York (1993).
7. P. Braunstein, L. A. Oro and P. R. Raithby (Eds.), *Metal Clusters in Chemistry*, Wiley-VCH, Weinheim (1999).
8. M. H. Chisholm (Ed.), *Early Transition Metal Clusters with π -Donor Ligands*, VCH, New York (1995).
9. J. D. Lee, *Concise Inorganic Chemistry*, Chapman and Hall, London (1991).

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Semester I

Organic Chemistry-I Paper Code: B02U0702T

Credits: 4

Unit 1: Reactive intermediates & Aromaticity

General methods of generation, detection, stability, reactivity and structure of the intermediates, Classical and non-classical carbocations and carbanions; radicals, radical cations, radical anions, carbenes, arynes and nitrenes, Aromaticity: Concept of aromaticity, benzenoid and non-benzenoid aromatic compounds

Unit 2: Stereochemistry

Molecular symmetry and chirality, stereoisomerism: definitions, classifications, configuration and conformation (R-S), Conformational analysis of n-Butane, cyclohexane and decalenes, optical activity in bi-phenyl, allenes and spiranes

Unit 3: Rearrangement and Reactions

Pinacol/Pinacolone Rearrangement, Wagner-Meerwein Rearrangement, Wolff Rearrangement, Hofmann Rearrangement, Curtius Reaction, Lossen Rearrangement, Schmidt Reaction, Beckmann Rearrangement, Favorskii Rearrangement and Claisen Rearrangements, Aldol Reaction, Perkin Reaction, Stobbe Reaction, Reimer-Tiemann Reactions.

Unit 4: Aliphatic, Electrophilic and nucleophilic substitution reaction

Nucleophilic (SN^1 & SN^2) substitution reaction, Electrophilic substitution reaction. Elimination reaction, Regioselectivity

Unit 5: Photochemistry of Carbonyl Compounds

Photo reduction of Ketone, Norrish Type I and II, photochemistry of α,β unsaturated ketones and cyclic ketones, Barton reaction and Hoffmann Loeffler Fretage reaction. Paterno Buchi reaction, olefin, Cis – Trans isomerism, dimerisation, Photochemistry of aromatic compounds: Rearrangement, isomerisation and addition to olefin. Photochemistry of Butadiene and Di- π -methane rearrangement, Photofries rearrangement.

Books Recommended:

1. Clayden, Greeves, Warren and Wothers, *Organic Chemistry*, Oxford University Press (2001).
2. M.B. Smith & Jerry March, *March's Advanced Organic Chemistry*, 5th Edition, John Wiley & Sons, New York (2001).
3. Peter Sykes, *A Guide book to Mechanism in Organic Chemistry*, 6th Edition, Orient Longman Ltd., New Delhi (1997).
4. S. M. Mukherjee and S.P Singh, *Reaction Mechanism in Organic Chemistry*, 1st Edition, Macmillan India Ltd., New Delhi (1990).
5. T.H. Lowry and K.S. Richardson, *Mechanism and Theory in Organic Chemistry*, 3rd Edition, Addison-Wesley Longman Inc. (1998).
6. G.S. Zweifel and M.H. Nantz, *Modern Organic Synthesis*, Freeman and Company, New York (2007).
7. M.S. Singh, *Advanced Organic Chemistry: Reactions and Mechanism*, Pearson Education (Singapore) Pvt. Ltd. (2005).

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Semester 1

Physical Chemistry-I Paper Code: B02U0703T

Credits: 4

Unit 1: Chemical Kinetics

Rate laws and temperature dependence, steady state approximation, kinetics of complex reactions, oscillatory reactions (Belousov- Zhabotinskii reaction), determination of reaction mechanism, collision and transition state theories of rate constant, Catalysis and enzyme kinetics, experimental techniques for fast reactions (stopped-flow, temperature-jump and flash photolysis).

Unit 2: Chemical thermodynamics

Thermodynamics properties: enthalpy, entropy, free energy, Partial molar properties in ideal mixture, chemical potentials, its determination and variation with temperature and pressure, Gibbs -Duhem equation. Fugacity and activity, variation with temperature and pressure, variation of Fugacity of a gas mixture, Duhem- Margules equation and its application. Le-Chatelier's principle, Phase equilibria and phase rule, thermodynamics of ideal and non-ideal gases and solutions.

Unit 3: Statistical Thermodynamics

Introduction: concept of ensembles, Thermodynamic probability, Boltzmann distribution law, Boltzmann Planck equation and its significance, Fermi-Dirac and Bose -Einstein distribution, Translational, Rotational, Vibrational and Electronics partition function, its application in the case of monoatomic and diatomic molecules.

Unit 4: Electrochemistry

Electrochemistry of solutions, Deby- Huckel – Onsager treatment and its extension, Metal / Electrolyte interface: OHP and IHP, potential profile across double layer region, potential difference across electrified interface; structure of the double layer: Helmholtz-Perrin, Gouy-Chapman, and Stern models.

Unit 5: Semiconductors(SC)/ Electrolyte Interface

Semiconductor (SC)/electrolyte interface: Creation of space charge region, capacity of space-charge, Mott-Schottky plots for n-type and p-type semiconductors, determination of flat-band potential and donor/acceptor densities, application of SC/electrolyte interface in solar cells.

Books Recommended:

1. J.O. M. Bockris and A.K.N. Reddy, *Modern Electrochemistry*, Vol.2A & B, 2nd Ed. Plenum Press, New York (1998).
2. E. Fermi, *Thermodynamics*, Dover Publications, New York (1956).
3. K. J. Laidler, *Chemical Kinetics*, 3rd Ed. Harper & Row, New York (1987).
4. P. W. Atkins and J. D. Paula, *Physical Chemistry*, 8th Ed., Oxford University Press, New York (2006).
5. Ira N. Levine, *Physical Chemistry*, 5th Ed., Tata Mc Graw Hill Pub. Co. Ltd., New Delhi (2001).
6. P.W. Atkins, *Comprehensive Physical Chemistry*, Oxford University Press, New York (2006).

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Semester I

Analytical Chemistry Paper Code: B02U0704T

Credits: 4

Unit 1: Basics of Filtration processes:

Introduction to unit processes and unit operations, Screening, Mixing, Coagulation and Flocculation, Sedimentation: Type of settling, Filtration for wastewater treatment. Types of filters -rapid sand filter, slow sand filter, high rate filter, pressure filter. Gravitational settling, Centrifugal impaction, Inertial impaction, Diffusion, Electrostatic precipitation,

Unit 2: Electron Microscopy:

Introduction, Principle and Instrumentation of Scanning Electron Microscope(SEM) and Transmission Electron Microscope (TEM).

Unit 3: Separation Techniques:

Solvent extraction (liquid-liquid extraction), general principles, relationship between extraction and distribution coefficient, distribution ratio, multiple extractions, extraction of metal organic complexes and ion association complexes.

Unit 4: Chromatographic Techniques:

Classification, basic principles and theory of chromatography, Paper and thin-layer chromatography: various techniques of development, visualization and evaluation of chromatograms, Ion-exchange chromatography: ion exchange process, synthesis and structure of ion-exchange resin, resolution, retention parameters, ion-exchange capacity.

Unit 5: Thermal Analysis:

Theory, methodology and applications of thermogravimetric analysis (TGA), Differential Thermal Analysis (DTA), and Differential scanning calorimetry (DSC). Principles, techniques and applications of thermometric titration methods.

Books Recommended:

1. Bassette and co-workers, *Vogel's Textbook of Quantitative Chemical Analysis*, Longman Group UK (1989).
2. C.N Banwell, *Fundamentals of Molecular Spectroscopy*, 4th Ed., McGraw Hill Education (2017).
3. M.H. Willard, L.L. Merrit, J.A. Dean, F.A. Settle, *Instrumental Methods of Analysis*, 7th Ed., CBS Publishers & Distributors (2004).
4. F.W. Fifield, D. Kaley, *Principles and Practice of Analytical Chemistry*, 4th Ed., Blackie Academic and Professional (1995).

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Semester 1

Inorganic Chemistry Practical Paper Code: B02U0705P

Credits:4

1. Qualitative analysis of inorganic mixture salts containing six-radicals including rare element salts and interfering radicals.
 - a) Qualitative analysis of acid radicals
 - b) Qualitative analysis of basic radicals
 - c) Qualitative analysis of interfering radicals.
2. Quantitative analysis
 - a) Estimation of chloride ion in water sample.
 - b) Estimation of copper in a solution of cupric salts.
 - c) Estimation of nickel by gravimetric analysis
3. Determination of total hardness of water.
4. Preparation of inorganic and coordination compounds and their characterization
 - a) hexaaminenickel(II)chloride
 - b) tetraamminecopper(II)sulphate monohydrate
5. Separation of the components by Paper chromatography
 - a) Mixture of amino acids
 - b) Mixture of sugars
 - c) Ortho & Para nitrophenol

Books Recommended:

- 1) I. M. Kolthoff, P. J. Elving and E. B. Sandell, *Treatise on Analytical Chemistry*, Pt-I, II, III, The Interscience Encyclopedia, Inc., New York (1959).
- 2) A. I. Vogel, *A Text Book of Quantitative Inorganic Analysis*, 3rd Ed., Longmans (1961).

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Semester II

Inorganic Chemistry-II Paper Code: B02U0801T

Credits:4

Unit 1: Chemistry of s and p block elements

Classification, synthesis, reaction, structure and bonding in Boranes, Nitrogens and Phosphorous compounds, Lipscomb's topological concept, styx rule, Wade's rules. Alkali metal complexes with macrocyclic ligands, Aqueous and complex chemistry of beryllium and aluminium.

Unit 2: Chemistry of d block elements

Synthesis, structure, reactions properties and bonding of 4d and 5d elements. molybdenum blue, tungsten blue, ruthenium blue, platinum blue, tungsten bronze, ruthenium red.

Unit 3: Chemistry of f Block Elements

Chemistry of Lanthanide: electronic configurations – oxidation states – Lanthanide contraction – its consequences – magnetic and spectral properties – occurrence, extraction and separation techniques, Use of lanthanides and their compounds.

Chemistry of Actinides: Synthesis of Trans uranium - electronic configurations – oxidation states position in the periodic table – actinide contraction – comparison of magnetic and spectral properties of actinides with those of lanthanides

Unit 4 : Organometallic Chemistry

Historical development, classification, nomenclature, valence electron count, oxidation number and formal ligand charge. 18-electron rule, concept of hapticity; synthesis, structure and bonding of homo and heteroleptic metal-carbonyls, nitrosyls, alkyls, alkenes, allyl, alkynes, and arenes.

Unit 5: Metal Clusters

Cages and metal clusters, Metal carbonyl clusters: skeletal electron counting, Wade-Mingos-Louher rule, Application of isolobal and isoelectronic relationships, capping rules, carbide, nitride, chalcogenide and halide containing clusters Cr, Re, Nb, Ta, Mo and W clusters, Cluster compounds in catalysis.

Books Recommended:

1. F. Basaloand R.G. Pearson, *Mechanism of Inorganic Reactions*, 2nd Ed., Wiley Eastern Ltd., New Delhi (1967).
2. D.F. Shriver and P.W. Atkins, *Inorganic Chemistry*, 3rd Ed., ELBS, London (1999).
3. F.A. Cotton and G.Wilkinson, *Advanced Inorganic Chemistry*, 6th Ed., John Wiley & Sons, New York (1999).
4. Keith F. Purcell and John C. Kotz, *Inorganic Chemistry*, W.B. Sauders Com., Hong Kong (1987).
5. Martin L. Tobe and John Burgess, *Inorganic Reaction Mechanisms*, 1st Ed. Longmans (1999).

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Semester II

Organic Chemistry-II

Paper Code: B02U0802T

Credits: 4

Unit 1: Addition to carbon-carbon multiple bonds

Addition to carbon-carbon multiple bonds: Addition reactions involving electrophiles, nucleophiles and free radicals, cyclic mechanisms. Orientation and reactivity, Hydrogenation of double and triple bonds

Unit 2: Pericyclic Reactions

Cycloaddition, Electrocyclic, Sigmatropic and Cheletropic reactions.

Unit 3: Heterocyclic synthesis

Introduction, synthesis and properties of Thiophene, Furan, Pyridine, Pyrrole, Quinoline and Indole.

Unit 4: Reagents in Organic synthesis

Grignard reagent, NaBH₄, LiAlH₄, Gilman's reagents, Lithium dimethyl cuprate, DDQ, oxidising agents: SeO₂.

Unit 5: Organic Synthesis

Disconnection approach (one and two group), C-C, C-X disconnection, 1, 3 and 1, 5-difunctional compounds.

Books Recommended:

1. Clayden, Greeves, Warren and Wothers, *Organic Chemistry*, Oxford University Press (2001).
2. M.B. Smith & Jerry March, *March's Advanced Organic Chemistry*, 5th Ed., John Wiley & Sons, New York (2001).
3. Peter Sykes, *A Guide Book to Mechanism Inorganic Chemistry*, 6th Ed., Orient Longman Ltd., New Delhi (1997).
4. G. S. Zweifel and M. H. Nantz, *Modern Organic Synthesis*, Freeman and Company, New York (2007).
5. S.M. Mukherjee and S.P. Singh, *Reaction Mechanism in Organic Chemistry*, 1st Ed., Macmillan India Ltd., New Delhi (1990).
6. T.H. Lowry and K.S. Richardson, *Mechanism and Theory in Organic Chemistry*, 3rd Ed., Addison-Wesley Longman Inc. (1998).
7. S.M. Mukherjee and S.P. Singh, *Pericyclic Reactions*, Mac Millan India, New Delhi (1980).
8. Jagdamba Singh and LDS Yadav, *Advanced Organic Chemistry/Organic synthesis*, Pragati Prakashan (2011).
8. I. Fleming, *Pericyclic Reactions*, Oxford University Press, Oxford (1999).

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Semester II

Physical Chemistry-II

Paper Code: B02U0803T

Credits: 4

Unit 1: Introduction to quantum mechanics

Postulates of quantum mechanics, Angular momentum and linear operator, Hermitian operators, properties of operators, Theorems of operators

Unit 2: Exactly soluble system

Linear harmonic oscillators, Harmonic vibration, Hermite differential equation and its solution through recursion relation polynomial, H- like atoms, Laguerre and associated polynomial, Legendre Polynomial equation and their solution

Unit 3: Approximate method, Huckel M. O. Theory and Chemical bonding

Variation method, secular equation, Slater determinant, Perturbation method, First order perturbation, Application to He-like atom, Symmetric and antisymmetric wave functions. Huckel theory of conjugate systems, bond order and charge density, its calculation, Application of ethylene, butadiene, allyl and benzene, LCAO- MO theory, application of LCAO-MO theory to H_2^+ ion and H_2 molecule.

Unit 4 : Symmetry and Group Theory

Symmetry elements and symmetry operation, definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes. Point symmetry group, Schonflies symbols, representations of groups of matrices, Character of a representation, The great orthogonality theorem (without proof) and its importance, Character tables and their use.

Unit 5: Colloids and Surfaces Chemistry

Stability and properties of colloids, Isotherms and surface areas, Bimolecular surface reactions: catalytic activity at surfaces, transition state theory of surface reactions, rates of chemisorption and desorption, unimolecular and bimolecular surface reactions, comparison of homogeneous and heterogeneous reaction rates, surface heterogeneity.

Books Recommended:

1. Ira N. Lavine, *Quantum Chemistry*, Pearson Education India (2016).
2. R .K. Prasad , *Quantum Chemistry*, 4th Edition, New Age International Publishers, New Delhi (2010)
3. A.K. Chandra, *Introduction to Quantum Chemistry*, 4th Ed., Tata McGraw Hill (2017).
4. John S. rose, *A Course on Group Theory*, Dover Publications Inc. (2003)
5. J.C. Berg, *Introduction Interfaces and Colloids*, World Scientific Publishing Co. (2009).

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Elective Papers

Semester II

Environmental Chemistry Paper Code: B02U0804T

Credits:4

Unit 1: Introduction to Environmental Chemistry

Concept and scope of environmental chemistry, Environmental terminology and nomenclatures, Environmental segments, The natural cycles of environment (Hydrological, Oxygen, Nitrogen)

Unit 2: Atmosphere

Regions of the atmosphere, Reactions in atmospheric chemistry, Earth's radiation balance, Particles, ion and radicals in atmosphere; Chemistry of ozone layer.

Unit 3: Hydrosphere and Lithosphere

Hydrosphere: Complexation in natural water and waste-water, Micro-organisms in aquatic chemical reactions, Eutrophication, Microbiology mediated redox reactions.

Lithosphere: Inorganic and organic components in soil, acid-base and ion-exchange reactions in soil, micro and macro nutrients, nitrogen pathways and N P K in soil.

Unit 4: Chemical Toxicology

Toxic chemicals in the environments, Impact of toxic chemicals on enzymes, Biochemical effects of arsenic, cadmium, lead, mercury, carbon monoxide, nitrogen oxides, sulphur oxides.

Unit 5: Air and Water Pollution

Air pollution: Particulates, Aerosols, SO_x, NO_x, CO_x and hydrocarbon, Photochemical smog, Air-quality standards

Water Pollution: Water-quality parameters and standards: physical and chemical parameters, Dissolved oxygen, BOD, COD, Total organic carbon, Total nitrogen, Total sulfur, Total phosphorus and Chlorine, Chemical speciation (Pb, As, Hg)

Books Recommended:

1. G.W. Vanloon, S.J. Duffer, *Environmental Chemistry - A Global Perspective*, Oxford University Press (2000).
2. F.W. Fifield and W.P.J. Hairens, *Environmental Analytical Chemistry*, 2nd Ed., Black Well Science Ltd (2000).
3. Colin Baird, *Environmental Chemistry*, W.H. Freeman and Company, New York (1995).
4. A.K. De, *Environmental Chemistry*, 4th Ed., New Age International Private Ltd., New Delhi (2000).
5. Peter O. Warner, *Analysis of Air Pollutants*, 1st Ed., John Wiley, New York (1996).
6. S.M. Khopkar, *Environmental Pollution Analysis*, 1st Ed., Wiley Eastern Ltd., New Delhi (1993).
7. S.K. Banerji, *Environmental Chemistry*, 1st Ed., Prentice-Hall of India, New Delhi (1993).

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Semester II

Liquid State Paper Code: B02U0805T

Credits: 4

Unit 1: General Properties of Liquids

Liquid as dense gases, as disordered solids, some thermodynamics relations, internal pressure and its significance in liquids, Different types of intermolecular forces in liquids, different potential functions for liquid Classical partition function for liquid, Correspondence principles, Configuration integral, Configuration Properties

Unit 2: Theory of Liquid

Theory of liquid, Partition function method or model approach, Single cell model, Communal energy and entropy, LTD model, significant structure model

Unit 3: Distribution Function and Related equation

Radial distribution function method, Equation of state in terms of RDF, Molecular distribution function, Pair distribution function, Relationship between Pair distribution and pair potential function, Cluster expansion

Unit 4: Supercool and Ionic Liquids

Theories of transport properties, Non Arrhenius behaviour of transport properties, Cohen – Turnbull free volume model, Configurational Entropy model, Glass transition in supercooled liquids.

Unit 5: Liquid Crystal

Introduction, classification, structure of liquid crystal forming compounds, chemical properties, applications.

Books Recommended:

1. P.A Egilstaff, *An Introduction to liquid state*, Academic Press (1994).
2. A.F.M Barton, *The Dynamic Liquid state*, Longman (1974).
3. T.L. Hill, *An introduction to statistical thermodynamics*, Addison Wiley (1960).
4. H. Eyring and M. S. John, *Significant liquid Structures*, ACS Publications (1961).

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Semester II

Organic Chemistry Practical Paper Code: B02U0806P

Credits: 4

1. Synthesis of Dibenzal acetone from benzaldehyde (Aldol condensation).
2. Preparation of 2,4-D (2, 4-dichlorophenoxyacetic acid).
3. Synthesis of p-nitroaniline from aniline.
4. Synthesis of anthranilic acid from phthalic anhydride.
5. Synthesis of p-aminoazo benzene from aniline.
6. Synthesis p-Chlorotoluene from p-toluidine.
7. Synthesis of p-nitroaniline and -bromoaniline.
8. Synthesis of ethyl n-butylacetoacetate by acetoacetic ester condensation.
9. Synthesis of Benzoyl propionic acid from succinic anhydride.
10. Cannizaro reactions: 4-chlorobenzaldehyde as substrate.

Books Recommended:

1. H. Middleton , *Systematic Qualitative Organic Analysis*, Adward Arnold (1939).
2. H. Clark, *Handbook of Organic Analysis*, Adward Arnold (1946)
3. A.R. Tatchell, *Vogel's Textbook of Practical Organic Chemistry*, 5th Ed., John Willey (1996).

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Semester II

Research Project Paper Code: B02U0807R

Credit: 8

Research project/ Industrial training and seminar

Dissertation / project report should be submitted and evaluated.

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Semester III

Applications of Spectroscopy

Paper Code: B02U0901T

Credits:4

Unit 1: Rotational and rotation-vibrational spectroscopy

Introduction, Principles, Instrumentation and Application of IR , FT-IR instrumentation, Raman spectroscopy: Raman Effect, rotational and rotation- vibrational Raman transitions, nuclear spin effects, polarization of Raman lines.

Unit 2: Electronic spectroscopy

Introduction, Principles, Instrumentation and Application of UV- Visible, Franck-Condon factor, solvent effects.

Unit 3: Nuclear Magnetic Resonance Spectroscopy

Introduction, Principles, Instrumentation and Application of NMR spectroscopy

Unit 4: Electron Spin Resonance Spectroscopy

Introduction, Principle, Technique, Instrumentation and Applications of ESR.

Unit 5: Mass Spectroscopy

Introduction, Principles, Instrumentation and Application of Mass spectroscopy

Books Recommended:

1. J. M. Hollas, *Modern Spectroscopy*, 4th Ed., John Wiley & Sons Ltd., Chichester (2004).
2. G. M. Barrow, *Introduction to Molecular Spectroscopy*, McGraw-Hill (1962).
3. C. N. Banwell and E.M. Mc Cash, *Fundamentals of Molecular Spectroscopy*, 4th edition, Tata McGraw Hill, New Delhi (1994).
4. A. Carrington and A. D. Mc Lachlan, *Introduction to Magnetic Resonance* , Chapman and Hall, London (1979).
5. J. M. Hollas, *Modern Spectroscopy*, 4th Ed., John Wiley & Sons (2004).
6. R. S. Drago, *Physical Methods in Chemistry*, W.B. Saunders Co., U.K. (1977)
7. R.M. Silverstein, G.C. Bassler & T.C. Morrill, *Spectroscopic Identification of Organic Compound*, John Wiley & Sons (1981).
8. E. A. O. Ebsworth, *Structural Methods in Inorganic Chemistry*, Blackwell Scientific Publications (1991).
9. W. Kemp, *Organic Spectroscopy*, 3rd Ed., W. H. Freeman & Co. (1991).

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Semester-III

Advance Principles of Physical Chemistry Paper Code: B02U0902T

Credits: 4

Unit 1: Advanced Electrochemistry

Introduction to electrochemistry: Nernst equation, electrode kinetics, dynamic electrochemistry, Butler-Volmer equation under near equilibrium and non-equilibrium conditions, exchange current density, Tafel plot, polarizable and non-polarizable interfaces. Overpotentials. Potentiostatic and galvanostatic electrochemical methods including chronoamperometry, coulometry, cyclic voltammetry and impedance spectroscopy.

Unit 2: Electrocatalysis

Definitions, Electrocatalytic potential, effect of electric field on electrocatalysis, Nanostructured and surface modified electrodes. Introduction to batteries, fuel cells and electrochemical solar cells. Electrochemical processes of particular relevance to energy conversion

Unit 3: Reactions in Solutions

Reaction between ions, effect of solvent (single & double sphere models), interpretation of frequency factor and entropy of activation, influence of ionic strength, salt effect, reactions involving dipoles, influence of pressure on reaction rates in solution, Molecular collisions

Unit: 4 Solid State

Crystals structures, Bragg's law and applications, Band structures of solids, defects in solids Perfect and imperfect crystals, intrinsic and extrinsic defects, point defects, line and plane defects, vacancies- Schottky defects and Frenkel defects, semiconductors: intrinsic and extrinsic (p-type and n-type), superconductors.

Unit 5: Non-equilibrium Thermodynamics

Difference between equilibrium and non-equilibrium thermodynamics, Criteria of non-equilibrium thermodynamics; Assumptions of non-equilibrium thermodynamics, uncompensated heat and its relation to other thermodynamic functions, Fluxes and forces relation between these two quantities, Entropy production in heat transfer, mass transfer in flow of current, in mixing of gases, and in chemical reaction; The Phenomenological equations: The linear laws, The Onsager relation, microscopic reversibility and Onsager reciprocity. Coupled reaction. Thermoelectric effects: Seebeck, Peltier and Thompson effect.

Books Recommended:

1. J. O. M Bockris & A. K. N. Reddy, *Modern Electrochemistry: Vol II*, Plenum Rosetta (2012).
2. C. Kalidas & M.V. Sangaranarayanan, *Non Equilibrium Thermodynamics: Principles and application*, Macmillan India Limited (2002).
3. A. J. Bard, L. R. Faulkner, *Electrochemical Methods: Fundamentals and Applications*, 2nd Ed. John Wiley and Sons (2001).
4. Piero Zanello, *Inorganic Electrochemistry: Theory, Practice and Applications*, 2nd Ed., Royal Society of Chemistry (2019).
5. S. R. de Groot and P. Mazur, *Non Equilibrium Thermodynamics*, Dover Publications Inc., New York (1984).

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6. I. Prigogine, *Introduction to Thermodynamics of Irreversible Processes*, 3rd Ed., John Wiley and sons (1968).
7. *Reaction Kinetics* (1998), M. J. Pilling and A.P.W, Seakins, Oxford Science Publication, New York
8. K.J. Laidler, *Chemical Kinetics*, 3rd Ed., Harper & Row Publishers, New York (1967).
9. J. Rajaram and J.C. Kuriacose, *Kinetics and Mechanism of Chemical Transformation*, 1st Ed. , MacMillan India Ltd., New Delhi (1993).
10. B. G. Cox, *Modern Liquid Phase Kinetics*, Oxford University Press, Oxford (1994).
11. R. D. Levine and R. B. Bernstein, *Molecular Reaction Dynamics and Chemical Reactivity*, Oxford University Press, Oxford (1987).

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**Elective Papers
Semester III**

Paper Code: B02U0903T

Bioinorganic, Nuclear and Supramolecular Chemistry

Credit: 4

Unit 1: Elements of Life

Roles of metal ions, Role of metal ions in medicine, Metal dependent diseases: Wilson's disease, Alzheimer disease, Metal complexes as drugs & mechanism: drugs. Toxic effects of metal ions, detoxification by chelation therapy.

Unit 2: Basic Reactions in Biological Systems

Bioenergetic principle and role of ATP, glucose storage, DNA polymerization, metal ion interaction with nucleoside and nucleotide; Photosynthesis, Chlorophyll, PS-I, PS-II, photosynthetic electron transport chain, cleavage of water, model system, nitrogen fixation.

Unit 3: Metal Ion Transport and Storage Proteins & Enzymes

Ferritin, transferrin, celluloplasmin, iron-sulphur protein (ferredoxin, rubredoxin), riske protein, Transport across biological membrane: $\text{Na}^+ - \text{K}^+ - \text{ATPase}$, ionophores. Oxygen transport & storage: haemoglobin(oxy-deoxy form), myoglobin, O_2 binding, partial pressure & Bohr effect, heamocyanin, hemerythrin, copper protein, model synthetic complex of Fe, Co, Cu. Hydrolytic enzymes: carbonic anhydrase, carboxypeptidase, urease. Protective metalloenzymes such as cytochromes, cytochrome P-450, superoxide dismutase, catecholase, peroxidase, nitorgenase, catalase, xanthine oxidase, Cobalamins including vitamin and coenzyme B12.

Unit4: Nuclear Chemistry:

Nuclear reactions, Fission and fusion reactions, Radio analytical techniques and activation analysis

Unit 5: Supramolecular Chemistry

Concept and definition, designing of building blocks, molecular supramolecular orbitals, polymeric ensembles (chain, sheet, network), supramolecular arrays: ribbon, ladder, rack, braded, grid; harnessing non-covalent forces (hydrogen bonding, pi-pi and C-H...pi interactions), lock and key principle, host-guest interaction to design functional materials, molecular machine.

Books Recommended:

1) A. Das and G. N. Mukherjee, *Elements of Bioinorganic Chemistry*, 2nd Ed., U. N. Dhur and Sons, Kolkata (2002).

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- 2) I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, *Bioinorganic Chemistry*, Viva Books Pvt. Ltd., New Delhi (1998).
- 3) W. Kaim and B. Schwederski, *Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life*, Wiley, New York (1994).
- 4) S. J. Lippard and J. M. Berg, *Principles of Bioinorganic Chemistry*, University Science Books, Mill Valley, CA (1993).
- 5) P. M. Harrison and R. J. Hoare, *Metals in Biochemistry*, Chapman and Hall (1980).
- 6) C. A. McAuliffe (Ed) *Techniques and Topics in Bioinorganic Chemistry*, Halsted, New York, (1975).
- 7) J. E. Huheey, E. A. Keiter and R. L. Keiter, *Inorganic Chemistry: Principles of Structure and Reactivity*, 4th Edn, Harper Collins College Publishers, New York (1993).
- 8) J. D. Lee, *Concise Inorganic Chemistry*, Chapman and Hall, London (1991).
- 9) R. W. Hay, *Bioinorganic Chemistry*, Ellis Horwood, Chichester, New York (1984).
- 10) J. W. Steed and J. L. Atwood, *Supramolecular Chemistry*, John Wiley and Sons, New York (2000).

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Semester III

Bio - Organic Chemistry

Paper Code: B02U0904T

Credits: 4

Unit 1: Carbohydrates

Introduction, Classification, Properties of Disaccharides and Polysaccharides (Maltose, Lactose, Sucrose, Cellulose, Starch etc.)

Unit 2: Amino acids & Protein

Amino acids Classification, Synthesis, Structure, Evaluation of protein quality, Peptide bond, denaturation of proteins, factors effecting denaturation, essential criteria for structure elucidation of protein, amino acid analysis, factors responsible for stabilization of secondary and tertiary structures.

Unit 3: Natural Products

A general introduction, isolation, synthesis and structure of Alkaloids: Nicotine, Morphine, Terpenoids: Camphor, Menthol, Steroids: Cholesterol and Ergocalciferol, Flavonoids: Quercetin and Kaempferol.

Unit 4: Vitamins

Properties, Occurrence, Structure and importance of Vitamins; fat soluble and water soluble vitamins.

Unit 5: Nucleic acid

Introduction, Nucleic Acids: Nucleosides, Nucleotides, Biological importance of nucleotides and pentose sugar structure and properties of uracil, thymine, guanine, cytosine, adenine. Structures of different forms of RNA, DNA (Watson and Crick Model), Concept of gene, Nucleic acid metabolism – central dogma, features of genetic code, A brief introduction of replication, transcription and translation.

Books Recommended:

1. F.A. Carey, & R.J. Sundberg, *Advanced Organic Chemistry*, Parts A & B, Plenum: U.S. (2004).
2. W. Carruthers, *Modern methods of Organic Synthesis*, Cambridge University Press (1971).
3. S. Warren, *Organic Synthesis: The Disconnection Approach*, John Wiley & Sons (1984).
4. J. March. *Advanced Organic Chemistry, Reaction Mechanisms and Structure*, John Wiley (2013).
5. W. Carruthers, *Some Modern Methods of Organic Synthesis*, Cambridge University Press (1987).
6. I. L. Finar, *Organic Chemistry*, ELBS, U.K. (1968).
7. R.T. Morrison & R. N. Boyd, *Organic Chemistry*, 7th Ed. Prentice Hall India (2010).
8. J. Clayden, *Organic Chemistry*, 2nd Ed., Oxford University Press (2012).

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Semester III

Nano Chemistry Paper Code: B02U0905T

Credits:4

Unit1: Introduction

Definitions and course organization, Historical development of nanomaterials , Classification of nanomaterials

Unit2: Preparation of nano particles

Top down and bottom up approach, electrochemical, chemical, photochemical and biochemical synthesis of nano particles.

Unit3: Structure and Bonding in Nanomaterials

Chemical Bonds (types and strength) Intermolecular forces, Molecular and Crystalline structures, Hierarchical structures, Bulk to surface transition, surface reconstruction, self assembly and thermodynamics

Unit 4: Properties & Characterization

Size dependence of properties Chemical Optical, vibrational, thermal, electrical, magnetic ,mechanical, theoretical Aspects-e.g. density functional theory, Scanning and Transmission Electron Microscopy, Scanning Probe Microscopies: Atomic Force, scanning tunneling microscopy Diffraction and scattering techniques, Vibrational spectroscopy, Surface techniques

Unit 5: Applications

Nano-electronics, Nano optics, Nanoscale chemical- and bio-sensing, Biological/bio-medical applications, Photovoltaic, fuel cells, batteries and energy-related applications, High strength nanocomposites , Nanoenergetic materials.

Books Recommended

1. T. Pradeep, *NANO: The Essentials*, Tata-McGraw Hill, New Delhi, 2007.
2. D. W. Bruce and D. O'Hare, *Inorganic Materials*, John Wiley and Sons, New York, 1992.
3. C. M. Sorensen, *Magnetism in Nanoscale Materials in Chemistry*, Wiley Interscience, New York, 2001.
4. K.J. Klabunde, *Nanoscale Materials in Chemistry*, Wiley-interscience, 2001
5. Bharat Bhushan (Ed.) *Springer Handbook of Nanotechnology*, Springer, 2007
6. C.P. Poole, and F.J. Owens, *Introduction to Nanotechnology*, Wiley India, 2006
7. G.A. Ozin, C. Andre, and L. Arsenault, Cademartiri, *Nanochemistry: A chemical Approach to Nanomaterials*, Royal Society of Chemistry, 2005
8. K. J. Klabunde, *Free Atoms, Clusters and Nanoscale Particles*, Academic Press, New York, 1994.

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Semester III

Pharmaceutical Chemistry Paper Code: B02U0906T

Credit : 4

Unit 1: Basics of Pharmaceutical Chemistry

Introduction: Characteristics of drug, Common drug targets, Efficacy, inhibitory concentration, lethal dose, therapeutic index, half life, pass time and frequency of dosing, agonists, antagonists, competitive and non competitive inhibitors

Unit 2: Drug Synthesis and Testing Techniques

In vitro testing, Line-Weaver-Burk Plot, Pharmacokinetics and pharmacodynamics, ADME, biological testing, natural and synthetic lead compounds, combinatorial synthesis, stereochemistry considerations and optimizing reactions

Unit 3: Structure - Activity Relationships

Quantitative structure-activity relationships, Pharmacophore: skeletal and non-skeletal, substrate based drug design and target based drug design, Case study

Unit 4 Antibiotics

Synthesis of selected antibiotics, Structure, activity, resistance issues, Different classes of antibiotics: Cephalosporins, Penicillins and other beta lactam antibiotics, Fluoroquinolones and other synthetic antibiotics

Unit 5: Advanced Therapeutics Techniques and importance

Strategies in design of Anticancer and anti-HIV drugs, Cytotoxicity and bioavailability issues, Drug delivery systems, Gene therapy, Immunotherapy, Important Drug Categories: Psychoactive drugs and cardiovascular drugs

Books Recommended:

1. D.A. Williams, , T.L. Lemke, , Foye's Principles of Medicinal Chemistry, Lippincott Williams and Wilkins (2005).
2. A. Kar, Medicinal Chemistry, New Age International Publishers (2007).
3. A. Gringauz, Introduction to Medicinal Chemistry: How drugs act and why? John Wiley and Sons (1997).

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Semester-III

Physical Chemistry Practical Paper Code: B02U0907P

Credits: 4

1. Saponification of ethyl acetate with sodium hydroxide by chemical method.
2. Comparison of acid strengths through acid catalyzed methyl acetate hydrolysis.
3. Energy of activation of acid catalyzed hydrolysis of methyl acetate.
4. Distribution coefficient of (i) Acetic acid
(ii) I_2 between two immiscible solvents.
5. Conductometric titration of a weak acid with strong base.
6. Conductometric titration of a mixture of weak and strong acids.
7. Water equivalent of calorimeter and determination of
(i) Heat of solution of potassium nitrate
(ii) Heat of neutralization of strong acid and strong base
(iii) Basicity of polybasic acids
8. Conductometric titration of KCl with $AgNO_3$.
9. Molecular weight of a non-electrolyte by cryoscopy method.
10. Acid-base titration in a non-aqueous media using a pH meter.
11. Determination of activity and activity coefficient of electrolytes.
12. Determination of rate constant for hydrolysis/inversion of sugar using polarimeter.

Books Recommended:

1. M. James and F.E. Prichard, *Practical Physical Chemistry*, London, Longman (1981).
2. R.C. Das and B. Behera, *Experimental Physical Chemistry*, Tata McGraw Hill (1983)
3. B.P. Levitt, *Findley's Practical Physical Chemistry*, Longman (1973).
4. J. C. Ghosh, *Experiments in Physical chemistry*, 1st Ed., Bharati Bhavan (1974).
5. D.P. Shoemaker, C.W. Garland and J.W. Niber, *Experimental Physical Chemistry*, 6th Ed. McGraw Hill (1998).

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Elective Papers

Semester IV

Advanced Organic Chemistry Paper Code: B02U1001T

Credits:5

Unit 1 Advanced organic synthesis:

Disconnection approach, one group and two group disconnections, reversal of polarity, chemoselectivity, one group C-C disconnection, two group C-C disconnections, 1,3-difunctional and 1,5-difunctional compounds. Tandem reactions, Domino reactions and multi-component reactions.

Asymmetric synthesis: Development of methodologies for asymmetric synthesis, regioselectivity, stereoselectivity, diastereoselectivity and stereospecificity. The chiral pool; chiral auxiliaries, reagents and catalysts; Diels-Alder reaction, alkylation of chiral enolates; dihydroxylation. Heck reaction. Reagent controlled methods – Use of chiral reagents – Asymmetric oxidation – Sharpless epoxidation – Asymmetric reduction – Use of lithium aluminium hydride and borate reagents.

Unit 2 Modern organic reactions:

Baylis-Hillman reaction, Henry reaction, Sakurai reaction, Tishchenko reaction, Ugi reaction. Brook rearrangement; Tebbe olefination. McMurry, Heck, Suzuki, Negishi, Sonogashira, Kumada, Stille, Hiyama, Buchwald-Hartwig, etc. Olefin metathesis.

Unit 3 Modern Reagents and organometallic chemistry:

Phosphorus, Sulphur and nitrogen ylides: Preparation, applications in organic synthesis and mechanism. Umpolung reactions (sulphur compounds, nitro compounds, lithiated ethers and related compounds). Principles and applications of phase transfer catalysis, crown ethers and polymer-supported reagents in organic synthesis.

organo-Li, -Cu, -Zn, -Cd, -Hg and -Pd compounds; metallocenes (Fe, Ru, Os); carbene and carbyne complexes. Organoboranes: Hydroboration, Preparation of Organoboranes, Reagents: Disiamyl borane, tetryl borane, 9-BBN, dicyclohexyl borane, mono- and di-isopinocampheyl boranes.

Unit 4. Organic spectroscopy:

NMR; 3J variation with dihedral angle, fused rings, spreading out effect, vicinal coupling in other ring sizes, geminal coupling; shapes of NMR signals, pi contribution, NOE; 2D-NMR, EI-MS, MALDI-TOF-MS. Mass Spectrometry: Introduction and fragmentation, Base peak, Molecular ion peak, Meta stable ion peak, α -cleavage bond, allylic bond cleavage and Mc Lafferty rearrangement, examples of mass spectroscopy of some organic compounds. UV-Visible Spectroscopy: applications in conjugated dienes, some correlation studies, trienes, polyenes, Woodward Fischer rule, α , β -unsaturated carbonyl compound, solvent effect, applications in aromatic and heterocyclic compounds. IR Spectroscopy: Concept of vibrational spectra, stretching and bending vibrations, application identification of functional groups Structural elucidation of Organic compounds by a combined application of the UV, IR, NMR and MASS spectral data.

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Unit 5. Medicinal Chemistry:

Drugs: Introduction, classification of drugs, brief discussion of drug targets, drugs based on enzyme inhibition: Drug design and synthesis of Drugs, Sulfa drugs, aspirin, paracetamol etc., Drug targets on nucleic acids, Definition of antagonist, agonist, prodrugs, pharmacokinetics and pharmacodynamics, Concept of structure-activity relationship (SAR) and quantitative structure and relationship (QSAR).

Books Recommended:

- 1) R. Noyori, Asymmetric Catalysis in Organic Synthesis, John Wiley, 1994.
- 2) W. Caruthers, Modern Methods of Organic Synthesis, 3rd Edn., Low Price Edition, Cambridge University Press, 1996.
- 3) F.A. Carey and R.J. Sundberg, Advanced Organic Chemistry, Parts A and B, 4th Edn., Plenum Press, 2001.
- 4) H. Budzikiewicz, C. Djerassi and D.H. Williams, Mass Spectrometry of Organic Compounds, Holden-Day, 1967.
- 5) N. S. Bhacca, S. Norman and D. H. Williams, Application of NMR Spectroscopy in Organic Chemistry, Holden-Day, 1964.
- 6) D. H. Williams and I. Fleming, Spectroscopic Methods in Organic Chemistry, 5th Edn., Tata McGraw-Hill, New Delhi, 2005.
- 7) W. Kemp, Organic Spectroscopy, 3rd Edn., McMillan, Hong Kong, 1991.
- 8) R. H. Crabtree, The Organometallic Chemistry of Transition Metals, 2nd Edn., John Wiley, 1994.
- 9) J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, Oxford University Press, Oxford, 2001.
- 10) S. Warren, organic synthesis the disconnection approach, john wiley & sons(asia) pte ltd, Singapore, 2004.
- 11) G. Thomas, Medicinal Chemistry – An Introduction, John Wiley, 2001.

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Semester IV

Advance Physical Chemistry

Paper Code: B02U1002T

Credit :5

Unit 1 Kinetics of Condensed Phase Reaction:

Factors determining reaction rate in solution, Transition state theory in solution, kinetics of ionic reaction, Dependence of rate constant on ionic strength and dielectric constant of medium, Bronsted- Bjerrum equation, study of fast reactions: Flash Photolysis, relaxation techniques, Molecular beam and shock tube kinetics, stop flow method.

Unit 2 Transition state theory:

Application of statistical mechanics to transition state theory, comparison of transition state theory with experimental results, thermodynamic treatment of TST, theories of unimolecular reactions - treatments of: Lindmann, Hinshelwood, Rice- Ramsperger- Kassel (RRK), and Rice- Ramsperger-Kassel-Marcus (RRKM).

Unit 3 Catalysis and Oscillatory behaviour:

Kinetics of catalytic reactions, Arrhenius Intermediates, Vant-Half intermediates, Theory of acid-base catalyst, Bronsted catalysis law, Hammett equation, Oscillatory reactions.

Unit 4 Kinetics of Electrodes:

Faradic and Non- Faradic current, rate law in faradic process, Current Density, Factors affecting electrode reaction, Effect of double layer structure on electrode reaction rates.

Unit 5 A) Corrosion : Scope and economics of corrosion, cause and types of corrosion, electrochemical theories of corrosion, Methods of protecting corrosion

B) Thermodynamics of Solids:

Specific heats of solids, Einstein heat capacity equation, Debye theory of Specific heat.

Books Recommended:

1. *Reaction Kinetics*(1998), M. J. Pilling and A.P.W, Seakins, Oxford Science Publication, New York
2. *Chemical Kinetics*, 3rd Edition (1967), K.J. Laidler, Harper & Row Publishers, New York.
3. *Kinetics and Mechanism of Chemical Transformation*, 1st Edition (1993), J. Rajaram and J.C. Kuriacose, MacMillan India Ltd., New Delhi.
4. *Modern Liquid Phase Kinetics*(1994), B. G. Cox, Oxford University Press, Oxford
5. *Molecular Reaction Dynamics and Chemical Reactivity*(1987), R. D. Levine and R. B. Bernstein, Oxford University Press, Oxford

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Semester IV

Advanced Inorganic Chemistry Paper Code: B02U1003T

Credits:5

Unit 1: Redox-Reaction Mechanism

Redox reactions: Classifications, kinetics and mechanism, outer-sphere reaction, self-exchange rate, electron tunneling hypothesis, heteronuclear redox reaction and simplified Marcus theory; Marcus cross relationship and its application, solvated electron; inner-sphere reaction, remote attack, doubly-bridged process, complementary and non-complementary redox reaction, ligand exchange, effect of bridging ligand in inner sphere reaction, intervalence electron transfer, induced reaction, electron-transport in metalloproteins

Unit 2: Catalysis in Inorganic Chemistry

homogeneous/heterogeneous catalysis: Wacker-Smidt synthesis, hydroformylation reactions, Monsanto acetic acid process, hydrogenation by Wilkinson's catalyst, water gas shift reaction (WGS), Fischer-Tropsch synthesis, alkene polymerization, hydrosilation, hydrophosphilylation, hydroamination, hydrocyanation and hydroboration reactions, Heck reaction, carbene catalysis. Metathesis: Grubb's 1st and 2nd generation catalyst, Olefin cross coupling metathesis (OCM), ring closing metathesis (RCM), ring opening metathesis (ROM), applications.

Unit 3: Photochemistry of Inorganic Complexes

Photoexcitation, fluorescence, phosphorescence, photosensitization, quenching, charge and energy transfer, excimer structure, prompt and delayed reaction, excited state of metal complexes, photo-substitution, photo-oxidation, photo-reduction, excited state electron transfer, reaction of bi-pyridine & phenanthroline complexes (Cr,Ru,Ir), comparison with organic compounds, metal complexes sensitizers, application of photochemical reaction of coordination compounds

Unit 4: Solid State Chemistry

Structure of NaCl, CsCl, ZnS, SiO₂, CaF₂, AlF₃, TiO₂. Bonding in metals, ionic, covalent and hydrogen bonded solids; Crystal defects, non-stoichiometric defects: perfect and imperfect crystals, intrinsic and extrinsic defects; point, line, and plane defects. Schottky and Frankel defects formation, Non stoichiometric defects, color centres in ionic crystals, electronic properties of solids, conductors, semiconductors, insulators, superconductors; ferroelectricity, antiferroelectricity, piezoelectricity, liquid crystals, cooperative magnetism.

Books Recommended:

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- 1) G. W. Parshall, Homogeneous Catalysis, Wiley, New York, 1980.
- 2) C. N. Satterfield, Heterogeneous Catalysis in Practice, McGraw-Hill, New York, 1980.
- 3) J. D. Atwood, Inorganic and Organometallic Reaction Mechanisms, 2nd Edn, VCH, New York, 1997.
- 4) F. Basolo and R. G. Pearson, Mechanism of Inorganic Reactions, 2nd Edn, Wiley, 1967.
- 5) F. A. Cotton, G. Wilkinson, C. M. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th Edn, John Wiley and Sons, Inc., New York, 1999.
- 6) B. Douglas, D. McDaniel and J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn, John Wiley and Sons, Inc., New York, 2001.
- 7) J. E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic Chemistry: Principles of Structure and Reactivity, 4th Edn, Harper Collins College Publishers, New York, 1993.
- 8) G. L. Miessler and D. A. Tarr, Inorganic Chemistry, Prentice-Hall, New Jersey, 1999.
- 9) 4) T. P. Fehlner, J. -F. Halet and J. -Y. Saillard, Molecular Clusters — A Bridge to Solid State Chemistry, Cambridge University Press, Cambridge, 2007.
- 10) G. Friedlander, E. F. Macias, J. W. Kennedy and J. M. Miller, Nuclear and Radiochemistry, Wiley Interscience, New York, 1981.
- 11) G. Choppin, J. O. Lilienzin and J. Rydberg, Radiochemistry and Nuclear Chemistry, ButterworthHeinemann, 2001
- 12) A. D. Kirk, Inorganic Photochemistry, Coord. Chem. Rev., 1981, 39, 225.

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Semester IV

Applications of Chemistry in Industries

Paper Code: B02U1004T

Credits:5

Unit 1: Cement, Ceramic and Glass

Composition of cement, mixing of cement clinker with Gypsum, Setting of cement. Composition, Physical and Chemical properties of Glass, Varieties of glass, Introduction to ceramics

Unit 2: Composites

Introduction, constituents of composites, Types, of composites, Microscopic and Macroscopic Composites, Dispersion, Strength, Particle and Fiber- reinforced Composites.

Unit 3: Fertilizers

N - Ammonia, Ammonium nitrate and Urea; P - Phosphoric acid, Single and Triple superphosphate, DAP; K- Potassium Nitrate and Muriate of potash.

Unit 4: Petrochemicals and Lubricants

Introduction, Occurrence, Composition of Petroleum, Natural gas, cracking, refining, octane rating, cetane number, flash and fire point determination. Lubricating oils and additives, Naphtha crackers and Profile of their products, Synthetic and Blended oils.

Unit 5: Paints

General characteristic, their function, Manufacture and Classification, Enamels, Emulsion paints, Water based paints. Formulation of paints: Function of vehicles, solvent, thinner, pigment, dyes, filler, resins, drier, insecticides, additives in paint formulation

Books Recommended:

1. Oliver Kahn, *Molecular Magnetism*, VCH Publishers, UK (1993)
2. W. D. Callisters, *Materials Science and Engineering: An Introduction*, Wiley (2006).
3. N. W. Aschcroft and N. D. Mermin *Solid State Physics*, Holt, Rinehart and Winston, New York (1976).
4. J. C. Anderson, K. D. Leaver, J. M. Alexander and R. D. Rowlings *Materials Science*. ELBS (2003).
5. Kelker and Hatz, *Hand Book of Liquid Crystals*, 2nd Ed. Wiley (2014).
6. V.C. Malshe and Meenal Sikchi, *Basics of Paint Technology, Part I & II* (2008),
7. G.P.A. Turner, *Introduction to Paint Chemistry*, Chapman& Hall (1967).

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Semester IV

Physical Methods in Chemistry Paper Code: B02U1005T

Credits: 5

Unit 1: Photoelectron Spectroscopy and Related Techniques:

Principle and applications to studies of molecules and surface. UPES and XPS. Auger electron and X-ray fluorescence spectroscopy (AES and XRF).

Unit 2: Electron Microscopy:

Introduction, Principle and Instrumentation of SEM and TEM.

Unit 3: Techniques for Studying Surface Structure

Low energy electron diffraction (LEED). Scanning tunneling and atomic force microscopy (STM and AFM).

Unit 4: X Ray Diffraction Method

Introduction, Bragg's law, Miller indices, Instrumentation and its applications.

Unit 5: Fluorescence techniques

Steady-state fluorescence spectroscopy. Time-resolved (Time correlated single photon counting-TCSPC) fluorescence spectroscopy. Introduction to Single molecule fluorescence and fluorescence imaging.

Books Recommended:

1. J.M. Hollas, *Modern Spectroscopy*, 4th edition, John Wiley and Sons, Chichester (2004).
2. C.N. Banwell and E.M. Mc Cash, *Fundamentals of Molecular Spectroscopy*, 4th Ed., Tata McGraw Hill, New Delhi (1994).
3. E.M. Mc Cash, *Surface Chemistry*, Oxford University Press, Oxford (2001).
4. A.K. Cheetham and P Day, *Solid State Chemistry Techniques*, Oxford Univ. Press, Oxford (1988).
5. Joseph R. Lakowicz, *Fluorescence Spectroscopy*, 2nd edition, Plenum Press, New York. (1999).

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Semester IV

Green Chemistry Paper Code: B02U1006T

Credits:5

Unit 1: Introduction Principle and Concepts of green Chemistry

Need for green chemistry, Inception and evolution of green chemistry, Twelve principles of Green Chemistry with their explanation and examples, Designing a green synthesis using these principles, Green chemistry in day to day life.

Unit 2: Non Traditional Greener Alternative Approaches

Different approaches to green synthesis: Use of green reagents in organic synthesis-Dimethyl carbonate, Polymer supported reagents- Peracids and Chromic acids, Green Catalysis , role of catalysis in sustainable development , homogeneous and heterogeneous catalyst, Introduction , advantages and applications of Biocatalyst.

Unit 3: Application of Non-conventional Energy Sources

Introduction of microwave induce synthesis: Microwave activation, equipment, time and energy benefits, limitations, Organic transformations under microwaves- Fries rearrangement , Diels -Alder reaction, Decarboxylation, saponification of ester.

Introduction of ultrasound assisted green synthesis: Instrumentation, Physical aspects, application in organic transformations.

Unit 4 Environmentally Benign Solutions to organic solvents:

Ionic liquids as green Solvents: Introduction, properties and types of ionic liquids, Synthetic applications- Diels -Alder reaction.

Aqueous phase reactions: Synthesis applications- 1,3- Dipolar Cycloadditions, Carbon-Carbon bond- forming processes and bromination reactions. Role of supercritical Carbon dioxide in green chemistry, Ethyl lactate as a renewable green solvent: Properties and applications.

Unit 5: Synthesis of Nanomaterials:

Greener synthesis of Nanomaterials –Magnetic Nanoparticles, MW assisted nano catalysis in water, Synthesis of Nanoparticles using Bacteria , Yeast, Algae and Fungus.

Books Recommended:

1. P.A.G. blackie , *Organic synthesis in water*, Springer (1998).
2. P.T. Anastas, *Green Chemistry : Theory and Practice*, Oxford University Press (2002).
3. M. Lancaster, *Green Chemistry : An Introductory Text* , Royal Society of Chemistry (2016)

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Semester IV

Photochemistry Paper Code: B02U1007T

Credits: 5

Unit 1: Photochemical Reactions

Introduction, types of excitations, fate of excited molecules, quantum yield, transfer of excitation energy

Unit 2: Determination of Reaction Mechanism

Classification, rate constant and life times of reactive energy state, determination of rate constant of reactions, effect of light intensity on the rate of photochemical reactions, types of photochemical reactions.

Unit 3: Photochemistry of Alkenes

Intramolecular reactions of olefinic bond- geometrical isomerism, cyclisation reactions, rearrangement of 1,4- and 1,5- diene.

Unit 4: Photochemistry of Carbonyls and Aromatic Compounds

Intramolecular reactions of carbonyl compounds, cyclic and acyclic $\beta\gamma$ saturated and $\alpha\beta$ unsaturated compounds, intermolecular cycloaddition reactions, Isomerization, additions and substitutions of aromatic compounds.

Unit 5: Miscellaneous Photochemical Reactions

Photo-fries reactions of anilides, Photo-fries rearrangements, Barton reactions, singlet molecular oxygen reaction, Photochemical formation of smog, photodegradation of polymers, photochemistry of vision.

Books Recommended:

1. N.J Turro, V. Ramamurthy, *Modern Molecular Photochemistry of Organic Compounds*, 10th Ed. University Science Books (2010)
2. B. Walder, *Principles and Applications of Photochemistry*, Wiley (2009).

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Semester IV

Material Chemistry Paper Code: B02U1008T

Credit :5

Unit 1: Introduction

Materials and their classification, inorganic and organic materials.

Unit 2: Inorganic materials

Design and synthesis of inorganic materials, requirements and constraints, combination properties of composites, functional materials, active materials; solid state reactions for synthesis of inorganic materials: ceramic methods, precursor method and sol-gel synthesis, physical and chemical vapour depositions; carbides, nitrides, structural and functional ceramics, intermetallics; intrinsic and extrinsic properties: electrical, optical and magnetic properties; ceramic superconductors, magnetic ceramics.

Unit 3: Organic materials:

Molecular electronics: molecular materials for electronics and molecular scale electronics: Molecular properties, molecular arrangement and molecular interactions, piezoelectric and pyroelectric organic materials; molecular magnets based on transition metal complexes and organic ferromagnets, organic non-linear optical materials: photochromic organic materials and their classes;

Unit 4: Conducting Materials

conducting polymers: polyacetylene, polypyrrole, polyaniline and polythiophene; conductive charge transfer materials: TTF- TCNQ, metal-dithiolate systems, fullerenes. Langmuir-Blodgett films, molecular electronic logic and architectures.

Unit 5: Applications of Inorganic, Organic and conducting materials

Books Recommended

1. P.J. Vander Put, *Inorganic Chemistry of Materials*, Plenum Press, New York, (1998).
2. M.C. Petty, M.R. Bryce and D. Bloor, Editors *An Introduction to Molecular Electronics*, Edward Arnold, London (1995).

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Semester IV

Paper Code: B02U1009T

Chemistry of Materials, Petrochemicals and Fertilizers

Credit :5

Unit I

Cement, Composites, Ceramic and Glass

Composition of cement, mixing of cement clinker with Gypsum, Setting of cement. Microscopic and Macroscopic Composites, Dispersion, Strengthened, Particle and Fiber- reinforced Composites. Composition, Physical and Chemical properties of Glass, Varieties of glass, Introduction to ceramics

Unit II

Magnetic and Nanomaterials

Ferromagnetism, Antiferromagnetism, Ferrimagnetism, Hysteresis, Remanence and Coercivity, Design of Molecular- based magnets: Three dimensional magnetic ordering. Preparation, Properties, Characterization and Applications of Nano materials (SEM, TEM).

Unit III

Fertilizers

N - Ammonia, Ammonium nitrate and Urea; P - Phosphoric acid, Single and Triple superphosphate, DAP; K- Potassium Nitrate and Muriate of potash.

Unit IV

Petrochemicals and Lubricants

Introduction, Occurrence, Composition of Petroleum, Natural gas, cracking, refining, octane rating, cetane number, flash and fire point determination.

Lubricating oils and additives, Naphtha crackers and Profile of their products, Synthetic and Blended oils.

Books Recommended:

1. Oliver Kahn. *Molecular Magnetism*, VCH Publishers, (UK).
2. W. D. Callisters. *Materials Science and Engineering: An Introduction*, Wiley.
3. N. W. Aschcroft and N. D. Mermin. *Solid State Physics*,
4. J. C. Anderson, K. D. Leaver, J. M. Alexander and R. D. Rowlings. *Materials Science*. ELBS.
5. Kelker and Hatz. *Hand Book of Liquid Crystals*

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Semester IV

Waste Management Paper Code: B02U1010T

Credit: 5

Unit I

Introduction and Types of Waste

Introduction to environmental Science. Definition, Types and Categories of Waste. Collection, Sorting and Transfer of waste, The Five R's.

Unit II

Solid and Liquid Waste Management

Techniques in Solid and Liquid waste Management. Waste Disposal and Scientific Landfill Cultivation. Municipal waste management

Unit III

Hazardous Waste Management

Introduction to Hazardous Waste Management (Nuclear waste and e-waste), Management and disposal of hazardous waste, Impact of Biomedical waste on environment and human health. Treatment and disposal of Biomedical waste.

Unit IV

Biomedical and Industrial Waste Management

Infection control, prevention and patient safety. Waste management in food industry, Reuse and recycling Techniques.

Entrepreneurship in waste management, Human Resource and Financial Management. Industry based case studies

Books Recommended:

1. Frank Kreith, *Hand Book of Solid Waste Management*, Mc Graw Hills, Newyork , 2017.
2. Yung-Tse Hung, *Hand Book of Environment and Waste Management voll*, World Scientific Publishing Company Pte Ltd. 2012.
3. John Pichtel, *Waste Management Practices; Municipal, Hazardous and Industria*, CRC Press, 2014.

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Semester IV

Polymer Chemistry Paper Code: B02U1011T

Credit: 5

Unit 1: Basic Concepts, Kinetics and Rheology

Polymers and their classification, nomenclature, Types of Polymerization: condensation, addition (free radical, cationic and anionic), copolymerization, Kinetics, Polydispersity and Molecular weight distribution, practical significance and measurement of molecular weight

Unit 2: Transition properties of polymer

Glass transition temperature in polymers (T_g), Melt transition (T_m), factors influencing glass transition temperature, relationship between T_g and T_m .

Unit 3: Polymer Degradation

Types of degradation: Thermal, Mechanical, photodegradation, degradation by radiation, oxidative and Hydrolytic degradation

Unit 4: Commercially Important Polymers and Applications

Commercially important Thermosetting and Thermoplastic polymers: Resins: Phenol Formaldehyde resins, Urea- Formaldehyde resins, Epoxy resins, Melamine- Formaldehyde resins.

Unit 5: Specialty Polymers

Biopolymers, Biomedical polymers, electrically conducting polymers.

Books Recommended:

1. J.R Fried, *Polymer Science and Technology*, Prentice-Hall of India (2000).
2. F.W. Billmeyer, *Textbook of Polymer Science*, Wiley-Interscience: New York (1984).
3. P.G. DeGennes, *Scaling Concepts in Polymer Physics*, Cornell University Press (1979).
4. R. J. Young & P. A. Lovell., *Introduction to Polymers* 2nd Ed., Champan & Hall (1991).

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Semester IV

Research Project Paper Code: B02U1012R

Credit: 8

Research project/ Industrial training and seminar

Dissertation / project report should be submitted and evaluated.

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