M.Phil. CHEMISTRY

CBCS Pattern 2019-2022

SPECIALIZATION PAPERS

1. SYNTHETIC ORGANIC CHEMISTRY

UNIT-I

Disconnection Approach

Importance of organic synthesis, comparison between linear and convergent syntheses. Retrosynthesis: Introduction to disconnection approach: Basic principles and terminologies used in disconnection approach. One group C-X and C-C disconnections. Retrosynthesis and synthesis of benzofurans, p-methoxy acetophenone and ibuprofen. Functional group transformations in organic synthesis - nitro to keto, nitro to amine and acid to alcohol.

UNIT-II

C-C and C-N bond forming reactions

Darzen's reaction, Use of acetylides in C-C bond formation reactions. Acid-catalyzed self condensation of olefins, Prins reaction, Shapiro reaction, Dieckmann cyclization, Robinson annulations, Hofmann-Loeffler-Freytag reaction. Hofmann-Martius reaction. Acyloin condensation. Houben-Hoesch reaction. Stork-enamine synthesis. Use of nucleophilic nitrogen and electrophilic carbon (NH_3, amines and nitrite as nucleophiles in substitution, NH_3 and amines in addition to ketones and aldehydes) and electrophilic nitrogen and nucleophilic carbon (nitration, nitrosation) for the bond formation reactions (Chichibabin reaction, Skraup synthesis).

UNIT-III

Oxidation, reduction and asymmetric synthesis

Cr (VI) oxidants, Mn (VII) oxidants, OsO_4, SeO_2, Pb $(OAc)_4$, HIO_4, Ag_2O, DMSO.

Ozone, peroxides (H_2O_2, *t*-BuOOH, dibenzoylperoxide) and peracids (CF_3COOOH, *m*-CPBA) as oxidizing agents.

Complex metal hydrides, dissolving metal reductions (including Birch, Benkeser, Clemmensen reductions), catalytic hydrogenation (homogeneous and heterogeneous), organoboranes as reducing agents. Wolf-Kishner reduction, McMurry reaction.

'*ee'* and methods of determination of '*ee'*. Stereoselectivity: classification, terminology and principle. Asymmetric synthesis and asymmetric induction.

UNIT IV

Green organic synthesis I

Introduction and need for green synthesis, basic principles of green chemistry. Green reagents-polymer supported reagents. Green catalysts, polymer supported catalysts, crown ethers. Biocatalysts – enzyme catalysed reactions – Bakers yeast. Green Chemistry for sustainable development. Green solvents, ionic solvents as green solvents, water as green solvent. Microwave assisted organic synthesis – principle, conventional Vs microwave heating, advantages-microwave assisted reactions-solvent free reactions-microwave assisted synthesis of heterocyclic compounds (synthesis of pyrimidine and pyridine derivatives)

UNIT V

Green organic synthesis II

Ultrasound assisted green synthesis - Introduction, instrumentation, the phenomenon of cavitation. Sonochemical esterification, substitution, addition, alkylation, oxidation, reduction and coupling reactions.

Multicomponent reactions – Introduction, Ugi reaction, Biginelli condensation, Mannich reaction, Hantzsch reaction, Passerini reaction, Strecker reaction, Nef reaction, Perkin reaction, Bischler Napieralski reaction, Friedlander reaction, Paul-Knorr reaction and Michael addition.

References:

1. Advanced organic chemistry, Jerry March, 4th Edn. John Wiley, 2008.

2. Designing organic synthesis: A disconnection approach, S. Warren, John Wiley & Sons, New York, 2nd Edn. 1987.

3. Introduction to organic chemistry, A. Streitweiser, Jr and C. H. Heathcock, Macmillan, 1985.

4. Modern synthetic reactions, H. O. House, W. A. Benjamin, California, 2nd Edn. 1972.

5. Some modern methods of organic synthesis, W. Carruthurs, Cambridge Univ. Press, London, 2nd Edn. 1978.

6. Organic reaction Mechanisms, 3rd Edn., V. K. Ahluwalia and R. K. Prashar, Narosa, New Delhi, 2005.

7. Paul Anastas and John Warner, Green Chemistry: Theory and Practice, Oxford University Press (2000)

8. V.K. Ahluwalia, Green Chemistry: Environmentally Benign Reaction, Third Ed., Ane Books Pvt. Ltd.

9. V.K. Ahluwalia, M. Kidwai, New Trends in Green Chemistry, Second Ed., Anamaya Publishers, New Delhi.

10. D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, New Age International, 1994

2. COORDINATION CHEMISTRY

Unit – I Basics of Coordination chemistry

Bonding theories of Coordination complexes**:** Crystal field theory – tetrahedral, square planar, square pyramidal, trigonal bipyrimidal, octahedral - applications and limitations; Spectrochemical series; Effect of ligand field strength on the colour of the complexes; John-Teller distortion; Molecular orbital theory – sigma and pi-bonding in metal complexes.

Electronic spectra and Magnetic Properties of metal complexes:

Ligand Field Spectra - Calculation of ligand field parameter, Russell-Saunders states, spin orbit coupling, Orgel diagram; Nephelauxetic effect; Charge transfer spectra - LMCT and MLCT; Magnetic properties of complexes; Optical properties - Luminescence and Phosphorescence.

Unit - II Geometries of Metal complexes

Complexes with coordination number two, three, four (tetrahedral and square planar complexes), five (trigonal bipyramidal and square pyramidal), six (octahedral and trigonal prism) and higher coordination numbers; Factors affecting the coordination numbers; Site preference in square planar and trigonal bipyramidal complexes; Isomerism in four and six coordination complexes.

Unit - III Characterization techniques

IR Spectroscopy: Identification of various functional groups in metal complexes; NMR Spectroscopy: Identification of protons or carbons in different environments; Mass spectrometry: Fragmentation pattern in complexes; ESR: Identification of geometry and

coordination number; Thermal studies: Uses of DTA and TGA in the stability of metal complexes; Single crystal XRD: Uses in the structural elucidation of metal complexes; Application of ORD and CD in the identification of complexes; Basic Computational studies: Gaussian for theoretical structural studies.

Unit - IV Metal complexes in biological systems - I

Porphyrin Systems: Structure and functions of Hemoglobin, Myoglobin and Chlorophyll; Metalloenzymes: Structure and functions of Blue copper proteins, oxidase, reductase, Superoxide dismutase (SOD), Carboxy peptidase-A, Carbonic anhydrase and Nitrogenase; Non-Heme iron-sulphur proteins: Ferridoxins, Rubredoxins and Cytochrome C.

Unit - V Metal complexes in biological systems - II

Nucleic acid structures: Types of binding modes of nucleic acids with metal complexes; Chemotherapy - Chelating Agents (with special reference to EDTA) and therapy based on in vivo chelation of radio nucleotides - Dosage and toxicity; Cis-platin and its mode of action, side effects; Radio diagnostic agents - MRI scanning, Gold containing Rheumatic agents and their mode of action – Lithium in Pschycopharmocoloical drugs.

References

1. Inorganic Chemistry - Principles of structure and reactivity, Fourth Edition, J. E. Huheey, E. A. Keiter and R. L. Keiter - Addition Wesley Publishing Co, NY, 1993.
2. Advanced Inorganic Chemistry - F. A. Cotton and G. Wilkinson
3. Mechanism of Inorganic reactions - F. Basolo and R. G. Pearson
4. Inorganic Chemistry - R. B. Heslop and P. L. Robinson
5. Introduction to Ligand Fields - B. N. Figgis - Wiley Eastern Ltd, New Delhi, 1976.
6. Bioinorganic Chemistry - I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine; University Science Books.

7. Dr Asim R Dass, Bioinorganic Chemistry 2007. Books and Allied (P) Limited.

8. Physical Methods in Bioinorganic Chemsitry - Lawrence Que,Jr.

9. Bioinorganic Chemistry: Inorganic elements in the chemistry of lie – Wolfgang Kaim, B. Schwederski.

10. Lawrence Que, Jr, Physical Methods in Bioinorganic Chemistry – Spectroscopy and Magnetism.

3. ORGANOMETALLIC CHEMISTRY

UNIT I

Classification of organometallic compounds – the metal carbon bond types –ionic bond – sigma covalent bond – electron deficient bond – delocalised bond –dative bond – metal carbonyl complexes – synthesis, structure and reactions – the nature of M-CO bonding – binding mode of CO and IR spectra of metal carbonyls – metal carbonyl anions – metal carbonyl hydrides– metal carbonyl halides – metal carbonyl clusters – Wades rule and isolobal relationship – metal nitrosyls – dinitrogen complexes – dioxygen complexes.

UNIT II

Metal alkyl complexes – stability and structure – synthesis by alkylation of metal halides, by oxidative addition, by nucleophilic attack on coordinated ligands – metal alkyl and 18 electron rule – reactivity of metal alkyls – M-C bond cleavage reactions– insertion of CO to M-C bonds – double carbonylation – insertions of alkenes and alkynes – insertions of metals with C-H bonds – alkylidene and alkylidyne complexes - reactivity of alkylidene and alkylidyne complexes. Alkene complexes – synthesis of alkene complexes by ligand substitution, by reduction and by metal atom synthesis – bonding of alkenes to transition metals – bonding in diene complexes – reactivity of alkene complexes – ligand substitution –reactions with nucleophiles – olefin hydrogenation – hydrosilation – Wacker process– C-H activation of alkenes – alkyne complexes – bonding in alkyne complexes –reactivity of alkynes – alkyne complexes in synthesis – cobalt catalysed alkyne cycloaddition.

UNIT III

Carbenes – carbene tranisition metal complexes – classification of carbene complexes – Fisher carbene complexes – structure and bonding in Fisher carbene complexes – Schrock carbenes – structure and bonding in Schrock carbine complexes transition metal complexes – N-heterocyclic carbenes – pincer N-hereocyclic carbenes activation – bond activation and catalysis of pincer NHC complexes — bridging carbenes – carbynes – Fisher carbynes complexes – structure and bonding in Fisher carbine complexes – Schrock carbynes – structure and bonding in Schrock carbynes complexes - nucleophilic and electrophilic attack on coordinated ligands – dehydrogenation reactions – amidation reactions – alkane activation – intramolecular and intermolecular C–H activation

UNIT IV

Cyclopentadienyl complexes – metallocenes – synthesis of metallocenes – bonding in metallocenes – reactions of metallocenes – CpFe/Cp2Fe+ couples in biosensors – bent sandwich complexes – bonding in bent sandwich complexes – metallocene halides and hydrides – metallocene and stereospecific polymerization of 1-alkenes – cyclopentadiene as a non-spectator ligand – monocyclopentadienyl (half-sandwich) complexes – synthesis and structures of allyl complexes – arene complexes – synthesis, structure and reactivity of arene complexes – multidecker complexes.

UNIT V

Homogeneous catalysis by transition metal complexes-Hydrogenation reactions – reversible cis-dihydro catalysts – monohydride catalysts –hydrogenation of alk-1-ene – asymmetric hydrogenation –role of metal complexes in Nobel Prize in chemistry- transfer hydrogenations – hydrosilation and hydroboration reactions – water gas shift reaction – reduction of carbon monoxide by hydrogen – hydroformylation of alkenes – alcohol carbonylation –

decarbonylation reactions – C-C cross coupling and related reactions – alkene oligomerisations and polymerizations – Zeigler-Natta polymerization – alkene dimerisation and oligomerisations – valence isomerisation of strained hydrocarbons – alkene and alkyne metathesis – oxidations of alkanes and alkenes – oxygen transfer reactions –supported homogeneous and phase transfer catalysis.

References

1. Organometallics I, Complexes with transition metal-carbon s-bonds, M. Bockmann, Oxford science publications, Oxford, 1996.

2. Organometallics II, complexes with transition metal-carbon p-bonds, M. Bockmann, Oxford science publications, Oxford, 1996.

3. Inorganic chemistry – Principles of structure and reactivity, J. E. Huheey, E.A.Keiter and R.L. Keiter, Addison-Wesley Publishing Company, New York, 2000.

4. Advanced Inorganic Chemistry, Sixth Edition, F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, John Wiley and sons, Inc, New York, 1999

5. Organometallic compounds, Indrajeet Kumar, Pragati edition, Meerut, 2010.

6. Organometallic Chemistry, R.C. Mehrotra, A. Singh, New Age International (P) Ltd, Publishers, Second Edition, 2000.

4. CORROSION CHEMISTRY

UNIT – I

Mechanism of electrode reactions – Polarisation and Over Potential – the Butler Volmer equation for one step and multi step electron transfer reactions – significance of equilibrium exchange current density and symmetry factor – transfer coefficient and its significance – Theory and applications of dropping mercury electrode – Polarography, Amperometry and Cyclic voltametry – Principles and applications – mechanism of Hydrogen and Oxygen evolution reactions.

UNIT – II

Electrochemical inorganic and organic reactions of technological interest – Corrosion and Passivation of metals – construction of Pourbaix and Evans diagrams – Prevention of Corrosion. Electrodeposition – Principles and applications.

UNIT III

Determination of corrosion and corrosion inhibition parameters – non-electrochemical methods: coupon – electrochemical resistance – gasometric methods. Electrochemical methods: polarization – galvanostatic-potentiostatic – potentio dynamic- AC impedance- hydrogen permeation.

UNIT – IV Electrochemistry of corrosion

Corrosion – introduction, definitions and types-Electrochemical cells-definitions and principles -Potential measurements - galvanic cells, concentration cells. -EMF and Galvanic series - bimetallic couples-Eh-pH diagrams – fundamental aspects - Construction of Eh – pH diagrams- FeH_2O-O_2 diagram- Copper, Aluminum and general corrosion diagrams.

UNIT – V Methods of corrosion control

Prevention strategies – design and coatings-Prevention strategies – inhibitors and surface engineering - Cathodic protection – principles and classification- Cathodic protection –

influencing factors and monitoring - Design aspects for cathodic protection-Stray current corrosion-Passivity – definitions and influencing parameters -Passivity – application of mixed potential theory-Passivity – design of corrosion resistant alloys-Anodic protection.

References

1. S. Glasstone, **Introduction to Electro Chemistry**, Affiliated East West Press, New Delhi, 1960.

2. D.R. Craw, **Principles and applications of Electro chemistry**, Chapman and Hall, 1991.

3. J. Robbins, **Ions in solution – An Introduction to Electro chemistry**, Clarendon Press, Oxford (1972).

4. J.O.M. Bockris and A.K.N. Reddy, **Electrochemistry**, Vols, 1 and 2, Plenum, New York. 1977.

5 R.H. Rieger, **Electrochemistry**, Chapmann and Hall, New York (1994).

6. P. Delahay, **Electrode Kinetics and Structure of Double Layer**, Interscience, 1965.

7. Branko N Popov**,** Corrosion Engneering.

8. Raj **Narayan**, ***Corrosion*** of metals and polymers

5. NANOCHEMISTRY

UNIT – I

Nanotechnology – Introduction- Importance- various stages of nanotechnology- nanostructures and nonmaterials. Techniques used in nanotechnology- Bottom up- self assembly- Top down fabrication techniques – EBL, DPN, NIL, UV lithography.

UNIT – II

Fabricationof nanoparticles – Grinding with ion balls-Gas condensation-Laser ablation-Thermal and ultrasonic decomposition-Reduction methods-Sol gel synthesis- Ceramic processing-Green and biological synthesis of metal nanoparticles- gold, silver and copper.

UNIT – III

Properties of nanoparticles– physicochemical properties – aggregation and disaggregation – surface properties – zeta potential – surface plasmon resonance – optical, thermal, mechanical,properties –quantum confinement – superparamagnetism.

UNIT – IV

Tools used in Nanotechnology – UV -Visible spectroscopy , FT-IR spectroscopy , Electron microscopy – SEM, TEM, AFM – dynamic light scattering, powder X-ray diffractometry and particle size analyser

UNIT – V

Application of nanoparticles: Agricultural, textiles, food, energy, environmental and biomedical applications. Nanoenergy devices – carbon nanotubes – nanofibres – nanocages – nanosensors.

REFERENCE BOOKS

1. W.R.Fahrner, *Nanotechnology and Nanoelectronics*, Springer (India) Private Ltd, 2006.
2. ManasiKarkare, *Fundamentals and applications of Nanotechnology*, I. K. International, 2008.
3. Y.S. Raghavan, *Nanostructures and Nanomaterials*, Arise Publishers & Distributors, 1st Editon2010.
4. T.Pradeep, Nano: The Essentials 8th reprint Tata-McGraw Hill Education Private Limited, 2012.
5. Aparna Bhattacharya, *Nanomedicine*, Rajat Publications, 2008.

6. ADVANCED MATERIALS CHEMISTRY

Unit-1 Fundamentals

General introduction about Nano science - Size and Scale, Units, Scaling, atoms, molecules, clusters and supramolecules. Structure and bonding in nanomaterial, chemical bonds (types and strength), intermolecular forces, molecular and crystalline structure, hierarchical structures, bulk to surface transition, surface reconstruction. Definition of nano structures – Emergence of nanotechnology – Historical perspective of nano materials, Classification of nano materials, Challenges in nanotechnology. Special Nanomaterials: Carbon nanotubes, fullerenes, nanowires, porous silicon.

Unit-II Synthesis

Fabrication of nanoparticles - Gas condensation-Thermal and ultrasonic decomposition. Reduction methods-Sol gel synthesis-Ceramic processing, Bio-inspired synthesis: Green and biological synthesis of metal nanoparticles - Gold, silver and copper. Thin films methods: Electrochemical deposition, Chemical vapor deposition, physical vapor deposition (Sputtering, Laser ablation), Galvanic deposition, Spin Coating, Langmuir-Blodgett growth. Mechanical methods: Ball milling, Mechanical attrition, Sol-gel, Microemulsion, Electrochemical, Wet chemical, template synthesis, mechanochemical synthesis and nanolithography. Advantages and Disadvantages of the methods.

Unit-III Characterization

Tools used in nanotechnology- UV- Visible spectroscopy, FT-IR spectroscopy-Electron microscopy- SEM,TEM, AFM, powder X-ray Diffractometry, X-ray Photoelectron Spectroscopy and Particle size analyser and Zeta potential determination, Photo luminescence spectroscopy, TGA/DTA, DSC.

Unit-IV Properties

Properties of Nanoparticles-Physicochemical Properties-Aggregation and disaggregation-Surface Properties-Zeta Potential, Surface Plasma Resonance-Optical Properties-Quantum Confinement, Magnetic, Mechanical, Thermal and Photocatalytic Properties.

Unit-V Applications

Nanotechnology in drug delivery, types of nanocarriers: nanogels, nanoparticles, nanoflims, nanofibres, nanosponges and nanoliposomes. Application of *In vitro* biological evaluation-bioactivity, biodegradation, biocompatibility, hemo biocompatibility, cell proliferation, cell apoptosis, cellular uptake, cell quantification and drug release kinetics. Applications of biomaterials- Fabrication and characterisation-Short term and long term applications in medicine.Nano-electronics, Nano optics, Nanoscale Chemical- Biosensing, Solar cells, Fuel cells, energy storage application.

Books/References:

1. C.N.R. Rao, A. Muller, A.K. Cheetham (eds), The Chemistry of nano materials synthesis, properties and applications, John Wiley- Vch-2001 Vol-2.
2. Challa S.S.R. Kumar Joset Hormes, Carola leuschner, Nano fabrication towards biomedical applications, John Wiley-Vch-2004.
3. Michael Kohler, Wolfgang Fritzsche, Nano Technology an introduction to nano structuring techniques, John Wiley-Vch-2003.
4. M.E. Muller, M. Allgower, R. Schneider, H. Willenegger, Manual of internal fixation techniques, Berlin Heidelberg, New York.
5. J. D. Currey, The mechanical adaptation of bones, Princeton university press, 1984.
6. H. Aoki, Science and medical application of hydroxyapatite, Japanise Associationof apatite science, Tokyo, Japan, 1991.
7. R.Z. Legeros, Calcium phosphates in oral Biology and medicine, karger, Basel, Switzerland, 1991.

8. B. O. Fowler, Structural properties of hydroxyapatites and Related compound, Gaithersburg, 1968.
9. Dr. H. Haur, Spectroscopy- K.K. Mitter, 2004 – 2005.
10. H.S. Randhawa, Modern molecular spectroscopy Rajiv-Beri – 2003.
11. Hobart H. Willard, Cynne C. Mesit Jr John A. Dean Frank, A. Settle Jr. Instrumental methods of analysis, sathish kumar-1986.
12. Robert M. Silverstein Francis X. Webster, Spectometric identification of organic compounds, Dr. G. Clayton Bassler – 1996.
13. C.N. Banwell, Molecular Spectroscopy, Tata Mc-graw hill, New Delhi-2004.
14. Douglas A. Skoog, Donald M. West F. James Holler, Fundamentals of analytical chemistry Harcourt Asia, Replika – 2001.
15. Douglas A. Skoog, F. James Holler, Timothy A. Nieman, Principle of instrumental analysis Thomson learning, Brooks/cole – 2004.
16. Manasi Karkare, Fundamentals and applications of nanotechnology, I.K. International, 2008.
17. Graphene-based materials and their composites: A review on production, applications and product limitations,Velram Balaji Mohanet.al, Composites Part B, (142) 200–220,2018.
18. Recent development of two-dimensional transition metal dichalcogenides and their applications,Wonbong Choiet.al,Materials Today, 20 (3), 116-130, 2017.

7. ENVIRONMENTAL CHEMISTRY

UNIT I Fundamentals

Concept and Scope of Environmental Chemistry; Origin and development of elements; Natural Cycles – Hydrological Cycle, Carbon Cycle, Oxygen Cycle, Nitrogen Cycle, Phosphorus Cycle, Sulphur Cycle; Natural and Man-made Disasters – Recent Natural Disasters; Anthropogenic Effects.

UNIT II Water Chemistry

Water chemistry- properties of water, nature of metal ions in water, solubility of gases in water, occurrence of chelating agents in water; Redox potential, Significance of redox equilibiria in natural and waste water; microorganisms; The catalyst of aquatic chemical reactions, water pollution and its effects, eutrophication concept of DO, BOD, COD, Sedimentation. Coagulation and filtration. Sampling techniques for water.

Unit III Wastewater Treatment

Wastewater treatment: Pretreatment – screening, grit removal and pre-chlorination; Primary treatment – settling and sedimentation; Secondary treatment – trickling filter process, activated sludge process; Aeration. Role of unit processes in waste water treatment chemical coagulation – Chemical precipitation for improved plant performance chemical oxidation – Neutralization – Chemical Storage.

Unit IV Industrial Wastewater Treatment

Industrial wastewater treatment: Activated sludge treatment plants – mass balances, with and without recycle plants; Types of plants – single tank, contact stabilization, biosorption plants.Biofilters: Hydraulic film diffusion, two component diffusion; Types of plants – trickling filters, submerged filters, rotating biological contractors and rotating disc; removal of particulate organic matter.

Unit V Treatment Plants

Treatment plants for nitrification – mass balances, nitrifying plants and types of plants.Treatment plant for denitrification - mass balances, denitrifying plants and types of plants; redox zones in the biomass. . – Microbial metabolism – Bacterial growth and energetics – Aerobic biological oxidation – Anaerobic fermentation and oxidation – Trickling filters – Combined aerobic processes – Activated sludge film packing .Plant types – pretreatment, plant with suspended sludge and filter process. Technologies used in advanced treatment – Removal of Colloids and suspended particles – Depth Filtration – Surface Filtration – Membrane Filtration Absorption – Ion Exchange – Advanced oxidation process.

REFERENCES

1. Sharma and Kaur, **Environmental Chemistry,** Krishna Publishers, New Delhi, 2000.
2. A.K. De, **Environmental Chemistry**, Wiley Eastern Ltd, New Delhi, 2014.
3. S.E Manahan, **Environmental Chemistry**, Lewis Publishers, London, 2001.
4. S.K. Banerji, **Environmental Chemistry**, Prentice Hall of India, New Delhi, 2005.
5. S.C.Bhatia, Environmental Chemistry, CBS Publishers, 2003.
6. J.Rose, **Environmental Toxicology**, Gordon and Breach Science Publication, New York, 1998.
7. S.M. Khopkar, **Environmental Pollution analysis**, Wiley Eastern, New Delhi, 1994.

8. POLYMER CHEMISTRY

Unit I Fundamentals

Importance, basic concepts, raw materials for polymers, concept of functionality, comparison of chain and step-growth, examples of polymerization reactions (polyadditions, polycondensations) constitution of polymers, homopolymers and copolymers, polymer architectures (graft copolymers, star-branched, hyperbranched and dendrimers), configuration and conformation of polymers, coil formation, mobility in polymers, glass transition temperature, rubber elasticity, molecular weight distribution,

Unit II Techniques of polymerizations:

Bulk, solution, suspension and emulsion polymerization techniques, melt polymerization, solid-state polymerization. Chemical Modification of Polymers: Cellulose modification- esterification and etherification of cellulose, natural rubber modification, cyclisation, hydrogenation and epoxidation of natural rubber. Polystyrene modification- hydrogenation, sulphonation, grafting and crosslinking of polystyrene.

Unit III Characterization techniques:

Fundamentals, experimental and applications to polymers of the following techniques: UV-visible spectroscopy, IR and Raman spectroscopy, Nuclear Magnetic (proton, carbon), resonance spectroscopy, NMR of polymers in the solid state, two dimensional NMR spectroscopy, pyrolysis GC-MS. X-ray diffraction, Transmission electron microscopy, scanning electron microscopy, thermal analysis (TGA, DTA, DSC), Dynamic mechanical analysis (DMA), electron spectroscopy for chemical analysis (ESCA).

Unit IV Polymer properties:

Approach and concept. Chemical structure of polymers- shapes and energy consideration, copolymers, heteroatomic polymers, molecular weight and distribution of molecular weights. Physical structure of polymers. Electrical and optical properties: Dielectric strength, dielectric

constant, volume resistivity, dissipation factor and loss factor. Optical properties: gloss, haze, yellowness index, transmittance and photoelastic Properties. Thermophysical properties of polymers in relation of chemical structures; Tg, Tm and relationships between Tg and Tm of polymer. The Crystallinity Polymers . Influence of molecular structure on mechanical, electrical, thermal and optical properties of polymers:

Unit V Functional Polymers:

Conducting polymers, polymeric reagents, polymer supports and catalysts, Photoresponsive Polymers, polymers in lithography Immobilization of Enzymes. Polymeric Materials for biomedical, engineering, agriculture, textiles, energy, environment, electronics, and defence applications

References

1. F.W. Billmeyer, TextBook of Polymer Science, 3rd Edition, J.Wiley, 2003.

2. V. R. Gowariker, N.V. Viswanathan and J. Sreedhar, Polymer Science, New Age Int., 1986.

3 H.R. Alcock and F.W. Lamber, Contemporary Polymer Chemistry, Prentice Hall, 1981.

4. P.J. Flory, Principles of Polymer Chemistry, Cornell University press, New York, 1953.

5. G. Odian, Principles of Polymerization, 2nd Edition, John Wiley & Sons, New York, 1981.

6.Jean-Pierre Farges, Organic Conductors, Marcel Dekkar, 1994

7.David B Cotts, Z Reyes, Electrically Conductive Organic Polymers for Advanced Applications, William Andrew Inc,1987

8. Larry Rupprecht, Conductive Polymers and Plastics, William Andrew Inc, 1999.

9. Raymond B Seymour, New Concepts in Polymer Science, Polymeric Composites, VSP, 1990.

10. Wallace Gordon, Gordon G Wallace, Geoffrey M Spinks, Conductive Electroactive Polymers, CRC Press, 2002

9. COMPUTATIONAL CHEMISTRY

UNIT I

Wave particle duality of matter – Louis de Broglie's theory. Heisenberg's uncertainty principle {principle of indeterminacy} – Formation of the New quantum mechanics - postulates quantum mechanics – simple harmonic Motion (SHM) – Wave mechanics –Schrodinger's wave equation – particle in one dimensional box – particle in three dimensional box

UNIT II

Term "computational chemistry "– its benefits and applications, methods of computational Chemistry-molecular mechanics, semiempirical, abinitio and Density functional theory (DFT) methods, Post hartree fock methods.

UNIT III

Writing a Z – matrix – basis sets and types – vibrational analysis – Finding TS, NMR analysis software's used in computation, Natural Bond Orbital analysis – current trends in computational chemistry, Output analysis

UNIT-IV

Combined QM/MM methods: Implications of the choice of QM and MM methods; Application of QM/MM methods in organic, inorganic and organometallic systems including bio-organic and bio-inorganic molecules. Quantitative structure activity relation (QSAR): Early approaches, topological indices, fragmental models; quantum mechanical descriptors

UNIT V

Benzenoid and Non-Benzenoid Aromatic compounds:-Introduction - structure of Benzene – Valence bond theory (Resonance theory) – molecular orbital theory – concept of aromatic character (Aromaticity) – theoretical criteria for aromaticity anti aromaticity – aromaticity and nuclear magnetic resonance – Non – benzenoid aromatic compounds

References

1. Frank Jensen (1999). *Introduction to Computational Chemistry*. England: John Wiley and Sons Ltd.
2. David Young ,*Computational Chemistry* , Wiley-Interscience, 2001
3. Jerry March, *Advanced Organic Chemistry*

10. SURFACE CHEMISTRY

Unit I

The Gas- solid inter phase,-types of adsorption. Heat of adsorption and its determination, differences between chemisorption and physisorption. Adsorption isotherms-classical, Freundlich and Langmuir isotherms. Thermodynamic and statistical derivation of Langmuir adsorption isotherm. Multilayer adsorption- the BET theory and Harkins- Jura theory.

Unit II

Adsorption from solutions: Gibb's adsorption equation and its verification. Adsorption with dissociation. Adsorption with interaction between adsorbate molecules. Different types of surfaces,Properties of surface phase. Thermodynamics of surface. Surface tension of solutions. Surfactants andmiscelles.

UNIT –III :

Micelles : Classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of Surfactants. Thermodynamics of micellization - phase separation and mass action models. Reverse micells, micro-emulsion. Micellar Catalysis, Surface tension capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets(Kelvin equation), Gibbs adsorption isotherm.

Unit IV

Examination of surfaces using low energy electron diffraction, photoelectron spectroscopy, ESCA, scanning probe microscopy, Auger electron spectroscopy , SEM and TEM. Surface films-different types, surface pressure and its measurement,surface potential and its measurements and interpretation. Measurement of surface area of solids - Harkins – Jura absolute method, entropy method . Use of Langmuir, BET and Harkins – Jura isotherms for surface area determination.

Unit V

Catalysis: Mechanism and theories of homogeneous and heterogeneous catalysis. Enzyme catalysis, bimolecular surface reactions. Langmuir – Hinshelwood mechanism, instrumental methods of catalyst characterization- diffraction and thermal methods, spectroscopic and microscopic techniques.

References

1,A.W.Adamson, “Physical Chemistry of Surfaces”, 5th edition Wiley India, 1990.

2 D.K.Chakrabarty and B. Viswanathan, Heterogeneous catalysis, New Age Publications, 2009.

3. G.A.Somorjai, Y.Li, Introduction to Surface Chemistry and Catalysis.International, 2nd edn., 2010.

4. Gurdeep Raj “Advanced Physical Chemistry” GOEL Publishing House, Meerut, 2004.

5. W.J. Moore, Physical Chemistry, Orient Longman, London, 1972.