BHARATHIAR UNIVERSITY::COIMBATORE – 46
M. Phil / Ph.D. - CHEMISTRY

PART I - SYLLABUS
(For the candidates admitted from the academic year 2018-19 onwards)

PART I: PAPER – I: RESEARCH METHODOLOGY

PAPER – II: PHYSICAL METHODS IN CHEMISTRY

PAPER – III: SPECIAL PAPERS

1. Environmental Chemistry
2. Polymer Chemistry
3. Organic Chemistry
4. Solid state chemistry.
5. Organometallic chemistry of transition metals.
6. Photochemistry-photophysical studies.
7. Physical organic chemistry
8. ElectroChemistry
9. Chemistry of advanced materials.
10. Organic Synthetic Methodology and Conformational Analysis

Note:

1. The syllabus for the above papers (Paper I, II and III Special Paper 6: Environmental Chemistry and Paper 10 : Polymer Chemistry) be the same as prescribed for the academic year 2009-10.

2. The syllabus for Paper I, II and III Special Paper 6: Environmental Chemistry and Paper 10 : Polymer Chemistry is furnished below.

PAPER – I: RESEARCH METHODOLOGY

UNIT - I

Dissertation: Nature and purpose, components and preparation- Writing techniques: Introduction, word processing and page layout, writing and formatting with a computer- Figures: general considerations, line art, drawing with a computer and halftones- Tables: logic behind a table, significance of a table, form of a table, components of a table - Worksheets, lists and databases. Plagiarism.

Collection and Citation of Literature:

Acquisition of information, building up of own literature collection, citation techniques, forms of citation, web of science, SCI, Scopus, H index and I10 index.

Publication of Journal Articles:

Concept, electronic publication, types of journals, impact factor, decision prior to publication, components of a journal article, preparation of the manuscript, from manuscript to publication and online submission.

Submission of Research Proposals:

Leading funding agencies in India, Submission of research project proposals with prescribed formats.

UNIT - II Data
Analysis:

Errors – classification of errors - precision - accuracy – improving accuracy of analysis – significant figures – mean, standard deviation – comparison of results: "t"test, "f" test and "chi" square test – rejection of results – presentation of data.

Sampling – introduction – definitions – theory of sampling – techniques of sampling – statistical criteria of good sampling and required size – stratified sampling *vs* random sampling – minimization of variance in stratified sampling –transmission and storage of samples.

UNIT - III

Atomic Spectroscopy and Flame emission Spectroscopy

Types of atomic spectroscopy – emission methods – absorption methods – fluorescence methods – atomizers for atomic spectroscopy: flame atomizers, Electrothermal atomizers – inductively coupled plasma sources of radiation – Instrumentation - Applications of atomic emission spectroscopy – flames and flame spectra.

Fluorometric analysis:

Types of Fluorescence and phosphorescence – factors affecting fluorescence and Phosphorescence – quenching – relation between intensity of fluorescence and concentration – measurement of fluorescence – applications.

UNIT - IV

Gas Chromatography:

Theory of chromatography – column efficiency and column equation – sample injection – sampling system for capillary columns and packed columns – detectors – gas flow control system – high resolution gas chromatography/mass spectrometry.

HPLC:

Principles of high performance liquid chromatography – Instrumentation - Pumps: types of pumps - requirements – Column packing : gradient elution, isocratic elution – Detectors for liquid chromatography – the mobile phase in HPLC – solvent degassing – column technology – column selection – quantitative analysis by HPLC-Applications.

UNIT-V Electroanalytical methods:

Redox potentials – definition – Methods of determination – applications – ion selective electrodes. Current – voltage relationships – polarography – instrumentation –Types of polarography– characteristics of DME – diffusion current – half wave potentials. Amperometric titrations - constant current coulometry – constant potential coulometry, cyclic voltammetry – basic principles and applications.

REFERENCES:

1. The art of Scientific Writing – H.F. Ebel, C. Bliefert and W.E. Russey 2nd ed Weinheim; Wiley-VCH (2004) .
2. R.C. Kapoor and B. S. Aggarwal - Principles of polography, 1st edition,Wiley (1991).
3. G. W. Ewing -Instrumental methods of chemical analysis,4th edition McGraw-Hill (1975).
4. Analytical electrochemistry- Joseph Wang, 2nd edition wiley (2001).
5. Instrumental methods of analysis – H.Willard, L.Merritt Jr.and A. Dean. 4th Edn(1996)
6. Instrumental methods of chemical analysis – B.K.Sharma., GOEL PUBLISHERS 28TH EDITION (2012).
7. Fundamentals of analytical chemistry – D.A.Skoog and D. M.West.7th Edu, Saunder s College Pub (1996)
8. Analytical chemistry – J.D.Dick. American Chemical Society (2007)
9. Basic concepts of analytical chemistry – S.M.Khopkar. New Age International, 1998**.**
10. Vogel's Textbook of Qualitative chemical analysis-5th edition.
11. Introduction of instrumental analysis (R. D.Braun,)(2009)
12. Principles of fluorescence spectroscopy – Joseph R.L**akowicz**,. 3rd edition Springer(2006).

PAPER-II: PHYSICAL METHODS IN CHEMISTRY

UNIT I

UV -Visible Spectroscopy:

Electronic excitation – origin of different bands – intensity of bands – selection rules - laws of photometry – correlation of electronic absorption with Molecular structure–chromophoric groups – conjugated systems – systems of extended conjugation– aromatic systems – empirical rules – experimental methods – photometric titrations.

IR - Spectroscopy:

Molecular vibrations – selection rules – force constant - band assignments – applications – organic structures – finger printing – identification of common functional groups – applications.

UNIT II

^{1}H and ^{13}C NMR Spectroscopy:

Proton chemical shifts – aromatic ring systems – anisotropic effects – ^{13}Carbon chemical shifts – mechanism of spin-spin coupling – vicinal, germinal and long range proton – proton coupling.

Analysis of NMR Spectra:

The energy level diagram – the selection rule – AB, ABC, AB and ABX spectrum- Pulse fourier transform techniques - Accumulation of spectra by the pulsed NMR technique – nuclear relaxation – fourier transformation - the pulsed FT NMR spectrometer.

UNIT III

Double resonance technique and relaxation mechanisms:

Homonuclear decoupling – heteronuclear decoupling – proton decoupling technique in ^{13}C spectrum- – INDOR and nuclear overhauser effect (NOE) – relaxation mechanisms – measurement of relaxation times - Spin-lattice relaxation (T_1) and spin – spin relaxation (T_2) measurements – assignment technique in ^{13}C spectra – 2D-NMR –COSY, HETCOR, NOESY, ROESY-DEPT. ^{13}C. Spectra-INADEQUATE, Spectra chemical shift correlation – quantitative measurement in ^{13}C – NMR – relaxation reagents – intensity standards.

UNIT IV

ESR Spectroscopy:

Theory – instrumentation – derivative curves values – "g" shift – origin of hyperfine splitting –isotropic systems – anisotropic systems – anisotropic effect - zerofield splitting – Krammer"s degeneracy –applications to organic and inorganic systems – identification of free radicals.

UNIT V

Mass Spectrometry:

Theory – instrumentation – various types of mass spectrometers – magnetic focusing instruments – sample handling – production and reactions of gaseous ions – isotopic abundance – determination of rearrangements – use of mass spectrometry in the structural elucidation of organic compounds – mass spectra of compounds containing different functional groups.

REFERENCES:

1. Proton and ^{13}Carbon- NMR Spectroscopy – An Integrated Approach – R.J.Abraham and Loftus.Wiley 1st edition (1992).
2. Spectroscopy of Organic Compounds, P.S.Kalsi, New age international pvt ltd Publisher 6th edition (2007).
3. Spectrometric Identification of Organic Compounds – R.M.Silverstein, G.C.Bassler andT. C. Morril Wiley 4th edition 1991.
4. Physical Methods in Inorganic Chemistry – R.S.Drago (1968).
5. Physical Methods in Organic Chemistry – J.C. P. Schwarz(1964).
6. Applications of NMR Spectroscopy in Organic Chemistry – L. M. Jackman and S. Sternhell Elsevier 2nd edition (1969).
7. Applications of absorption spectroscopy of organic compounds – John. R.Dyer PHI learning 1st edition (2009).
8. Interpretation of Mass Spectra – F. W Mclafferty 2nd edition(1994)
9. Introduction to spectroscopy- Donald L Pavia Wadsworth Publishing Co Inc 2008
10. NMR of Organic Chemists – D. W. Mathieson. Academic press (1967).
11. Electron Spin Resonance – Elementary Theory and Practical Applications – John E.Wertz and James R.Bolton(1972).
12. Mass Spectrometry for Organic Chemists – R.A. W. Johnstone. Cambridge, (1972).
13. High Resolution NMR - Edwin Becker 3rd edition, Elsevier(1999)
14. Interpretation of Mass Spectra of Organic Compounds – Hamming and Foster 1st edition, Elsevier (1972)
15. Organic Spectroscopy by William Kemp, Macmillan, 1991.

PAPER-III – 1. ENVIRONMENTAL CHEMISTRY

UNIT-I – WATER POLLUTION:

1.1 : **Classification of water pollutants**: Unique characteristics of water – The different types of pollutants – Thermal pollution.

1.2. : **Heavy metalst**: Detection – estimation – effects of heavy metals – Mercury – Lead – Arsenic – Cadmium.

1.3 : **Soaps and Detergents**: The need – The Classification – The characteristics – Environmental impacts of Soaps and Detergents –Abatement procedures for soaps and detergents pollution.

1.4 : **Paper Mills**: Paper Manufacture – Environmental Implications of Paper Mills – Abatement of paper mills pollution.

1.5 : **Ground water Pollution**: Characteristics of ground water – Types of ground water pollution – sources of Ground water pollution –Environmental effects associated with ground water – ground water in Indian perspective – Mitigation of Ground Water pollution.

1.6 : **Water Treatment**: Water purification – criteria of water purity.

UNIT II – AIR POLLUTANTS

Introduction – definition – classification of air pollutants – air quality standards.

2.1 : **Sulfur Oxides**: Sources of Sulfur oxides – Fate of sulfur oxides in the Environment – Analysis of sulfur oxides – Effects of Sulfur Oxides – control measures for sulfur oxides.

2.2 : **Nitrogen Oxides**: Sources of Nitrogen Oxides – Fate of Nitrogen oxides in the Environment – Analysis of Nitrogen Oxides Effects of Nitrogen Oxides – Control Measures for Nitrogen Oxiles.

2.3 : **Carbon Monoxide**: Sources of Carbon Monoxide – Fate of Carbon Monoxide in the Environment – Analysis of carbon Monoxide – Effects of Carbon Monoxide – Control Measures for Carbon Monoxide.

2.4 : **Photochemical Smog**: Formation of Photochemical smog – Effects of Photochemical smog – Control of potochemical smog.

2.5 : **Green House Gases**: The Green house effect – Causes of green house effect – consequences of Green house effect – Abatement of Green house effect – Tie-in-strategies – The Kyoto Protocol.

2.6 : **Depletion of Stratospheric Ozone**: Introduction – Mechanism of Ozone Depletion – Causes of Ozone Deplation – Consequences of Ozone Depletion – Abatement of Ozone Depletion – The Montreal Protocol.

2.7 : **Suspended Matter**: Types of particulates – Sources of particulates – Fate of particulates in the Environment – Analysis of particulates –Effects of particulates – Control Measures for particulate pollution.

2.8 : **Hydrocarbons**: Characteristics of Hydrocarbons – Sources of Hydrocarbons – Fate of Hydrocarbons in the Environment – Analysis of Hydro Carbons – Effects of Pollution by Hydrocarbons – Control measures for Hydrocarbons.

UNIT III – POLLUTANTS FROM INDUSTRY

3.1 : **Polymers and Plastics**: The Need – The classification – The characteristics – Environmental Implications of polymers and plastics – abatement procedures for polymers and plastics pollution.

3.2 : **Asbestos**: Structural characteristics of Asbestos – applications of asbestos – sources of asbestos in the environment – analysis of asbestos – effects of asbestos pollution – Mitigation of asbestos pollution.

3.3 : **Polychlorinated Biphenyls**: The need – Fate of poly chlorinated Biphenyls in the Environment – Environmental Implications of Polychlorinated Biphenyls – Abatement procedures for poly chlorinated Biphenyls pollution.

3.4 : **Food Additives**: The Need – The Classification – Risk Analysis of specific Additives.

3.5 : **Mining Operations**: Types of mining operations – Steps involved in mining operations – Environmental effects of associated with mining operations.

UNIT IV – POLLUTANTS FROM AGRICULTURE

4.1 : **Fertilizers**: The need – The classification – Environmental implications of fertilizers – Abatement procedures for fertilizers pollution – Eutrophication.

4.2 : **Insecticides**: The classification – The characteristics –Environmental implications of insecticides – Abatement procedures for insecticides pollution – Bhopal Episode.

4.3 : **Fungicides and Herbicides**: The need – The classification – The characteristics – Environmental Implications of Fungicides and Herbicides – Abatement procedures for fungicides and Herbicides pollution.

UNIT V – CHEMISTRY OF SOLID WASTE

5.1 : **Chemistry of Solid Waste**: Chemistry of composting; mechanism involved in the decomposition of organic materials like hemicelluloses, proteins, carbohydrates, food materials, organic insecticides, farm wastes, etc., by aerobic and anaerobic processes.

5.2 : **Chemistry of Incineration and Pyrolysis:**

Incineration: Definition – incineration of solid waste – combustion characteristics of various Inorganic and organic materials – heating values – determination of heating values of combustible liquid and solid wastes – air requirements for combustion – fate of trace constituents such as sulphur during incineration – gaseous pollutants, definition of phyrolysis – chemical changes taking place in organic and inorganic materials during pyrolysis importance of pyrolysis in the solid waste disposal; chemistry of recycling of solid wastes – recycling and reuse of materials such as paper, plastic, glass, etc.

REFERENCES:

1.Sawer, C.N. and PL. McCarty, „Chemistry for Environmental Engineers", Mc.Graw Hill, 1978.
2.Stumm, W. And J.J. Morgan, „Aquatic Chemistry". Wiley Interscience 1972.
3.American Public Health Association inc., New York, „Standard methods for the examination of water and waste water", 1976.
4.Stern, A.C., „Air Pollution", Vol. 1,2 and 3, Academic Press, New York 1968.
5.Strauss, W.Ed., „Air Pollution Control". Part 1,2 and 3, Wiley Interscience, New York, 1960.
6.Ross. R.D., „Air Pollution and Industry", V.N. Reinhold Co., New York, 1972.
7.Leithe, W. Translated by R. Kenor, „The Analysis of Air Pollutants", Ann Arbor, 1971.
8. Hagerty, D.J., J.L. Pavoni and J."E.Heer, Jr., „Solid Waste Management", Van Nostrand Reinhold Co., New York, 1973.
9. Wilsion,D.G. „Hand book of Solid Waste Management", V.R. Nostrand, Reinhold, New York, 1977.
10.De, A.K., Environmental Chemistry, New Age International Publishers Private Ltd., New Delhi, Fifth Edition, 2008.

11.Dara, S.S., Environmental Pollution and Control, S.Chand & Co., New Delhi, First Edition, 1993.
12.Sodhi, G.S., Fundamantal Concepts of Environmental Chemistry, Narosa Publishing House Pvt. Ltd., New Delhi, Third Edition, 2009.
13. Tyler miller Dr.G. ., Environmental Science, Cengage Leaching binate the new Delhi, Eleventh Edition ,2006.
14. Raghunath,H.M., Ground Water, Wiley Eastach Limated, New Delhi, Second Edition,1987.

PAPER – III: 2. POLYMER CHEMISTRY

UNIT - I

Step-reaction polymerization (condensation polymerization)

Chemical reactivity and molecular size, theory of reactivity of large molecules, kinetics of condensation polymerization, self catalyzed polymerization, external catalysis of polymerization, cyclization Vs linear polymerization, multi-chain polymerization and their molecular weight determination. Kinetics of degradation of Condensation polymers – hydrolysis of polyimides, hydrolysis of polyesters-interchange reactions in condensation polymers.

UNIT – II Radical Chain (Addition) Polymerization

Kinetics of chain polymerization – dependence of RP on initiator, monomer and temperature. Photo chemical initiation, thermal initiation, redox initiation, initiator efficiency, auto acceleration, kinetics of thermal polymerization. Kinetic chain length and degree of polymerization. Kinetics of chain transfer, chain transfer with monomer, solvents, Non-radical chain polymerization – cationic polymerization – mechanism and kinetics (General), anionic polymerization – kinetics and mechanism (General).

UNIT – III Co-ordination Polymerization

Definition of Ziegler- Natta catalysts, factors determining behaviour of catalysts, importance of physical state of the catalyst, soluble catalyst, colloidal catalyst, heterogeneous catalyst and supported catalysts. Proposed mechanism – monometallic mechanism, bi-metallic mechanism, experimental evidence. Mechanisms for stereochemical control of □-olefins – mode of addition, isotactic propagation, syndiotactic propagation. Industrial uses of co-ordination catalysts.

UNIT – IV Chain Structure and conformation of Polymers

Vibrational spectroscopy and nuclear resonance spectroscopy of polymers – polymethyl methacrylate, polystyrene-propagation statistics. Region regularity and branching in vinyl polymer chains – head-to-tail versus head-to-head; tail-to-tail (special evidence) isomerism – regioregularity – poly vinyl chloride, polyvinyl alcohol - branching in vinyl polymers – polyethylene, polyvinyl chloride - geometrical isomerism in diene polymers – Polybutadiene and polychloroprene (special evidence) solid state NMR of Polymers (General).

UNIT – V Speciality Polymers:

Polymeric liquid crystals- Main chain liquid crystal polymers, side chain liquid crystal polymers , examples and applications. Conducting polymers- Preparation, processing and applications of polyaniline. Photosensitive polymers – positive and negative photoresists, examples and applications. Heat resistant and flame retardant polymers – examples, mechanism and application. Polymer for biomedical applications – artificial organs, controlled drug delivery, haemodialysis and hemofiltration.

REFERENCES:

1.F.W. Bill Mayer, Text Book of Polymer Science‟ Wiley – Inter Science (1971).
2.H.R. Allcock and F.W. Larube, „Contemporary Polymer Chemistry‟ Prentice Hall (1981).
3.L.H. Sperling „Introduction to Physical Polymer Sciences‟ John Wiley & Sons (1986).
4.George Odian – „Principles of Polymerization‟ McGraw Hill Book Company (1970).
5.P.J. Flory – „Principles of Polymer Chemistry‟ Cormell Univ. Press (1953).
6.AD Ketley „The Stereochemistry of Macromolecules‟ Decker (1967).
7.Zbinder – „Infrared spectroscopy of High Polymers‟ Academic Press (1964).
8.K.J. Saunders „Organic Polymer Chemistry‟ – Capman Hall: (1973).
9.Randall –„Polymer sequence Determination Carbon – 13 NMR Method‟ Academic Press (1977).
10.Bovey F.A. „High Resolution NMR of Macromolecules‟ Academic Press (1972).
11.Joel R. Fried, "Polymer Science and Technology", 2nd Edn., Prentice Hall of India Pvt. Ltd., 2003
12. Progress in Polymer ScienceVol.34, pp 783 – 810, 2009 (ELSEVIER)
13.Arnost Reiser, "Photoreactive Polymers", John Wiley & Sons, 1989
14. Peter J. Collings, "Introduction to Liquid Crystals Chemistry and Physics", Chapter 5, Taylor and Francis, 1997.

PAPER – III: 3. ORGANIC CHEMISTRY

UNIT I

Pericyclic Reactions: Mechanism and synthetic applications of electrocyclic, cycloaddition (2+2 and 4+2) reaction and sigmatropic rearrangement. Explanation based on Frontier Molecular Orbital, correlation diagram and PMO approach.

UNIT II

Retro Synthesis: The disconnection approach – basic principles- synthons (acceptor and donor), synthetic equivalents– one group C – X disconnection – two groups C – X disconnection. Two group disconnections – Diels-Alder reactions – 1,3-difunctionalised compounds and α, β-unsaturated carbonyl compounds – 1,5-difunctionalised compounds, Michael addition and Robinson annulation – 1,2-, 1,4- and 1,6- difunctionalised compounds.

UNIT III

Organic photochemistry: Principles of Photochemistry and Photochemical reactions: [2 + 2] photochemical cycloaddition; Paterno-Büchi reaction; Photochemistry of cyclohexadienones, Norrish type I & II reactions. Photochemistry of enones and dienones: Photo Fries, di-π methane, oxa & aza di-π methane rearrangements.

UNIT IV

Modern reagents in organic synthesis: Sodium cyanoborohydride – Osmium tetraoxide – DABCO (1,4-diazabicyclo[2.2.2]octane), HMPA (Hexamethylphosphoramide), Lithium dialkylcuprate – Thallium trifluoroacetate – Sodium hydrogentelluride – Silver hexafluorantimonate – Thiobenzoyl chloride – Trichloro-

silane – Vanadium oxytrifluro – Hexachlorophosphazene – Ruthenium tetraoxide – Barium manganate – Benzene selenic acid – Benzene selenyl bromide/chloride, Aluminium chloride/Phosphoryl chloride.

UNIT V

Natural Products: Introduction, plant and animal based phytochemicals-basic biological importance of steroids, saponins, alkaloids, flavonoids, carotenoids, anthocyanins, terpenoids, lipids, proteins, glycosides and phenols.

Total Synthesis: Cecropia Juvenile Hormone, Marrubin, Buffalin, (+) – Lunacrine, Flindersine, geibalansine.

REFERENCES:

1. Organic Reactions & Orbital Symmetry – PL. Gilchrist & R.C. Storr.
2. The Conservation of Orbital Symmetry – Woodward and Hofman 4. 1,2 – Cycloaddition Reactions – Muller and J Hamer.
3. Roland E. Lehr and Alan P. Marchand, Orbital symmetry-A problem - solving approach.
4. Organic Synthesis through Disconnection Approach–P. S. Kalsi.
5. S. Warren, Designing Organic Synthesis – A Programmed Introduction to Synthon Approach, Wiley, NY, 1978.
6. Photochemistry and Pericyclic Reactions, 3rd Edition PB 3rd Edition by Jagdamba Singh and Jaya Singh.
7. Reagents for Organic Synthesis – Fisher & Fisher Volumes. I – XII.
8. Organic Chemistry Vol 2: Stereochemistry and the Chemistry of Natural products- I. L. Finar (5th edition).
9. Natural Products Chemistry Vol. I edited by Koji Nakanishi Tosti Ohto, Sboito, Shinsaku Natori and Shigeo Nozoe.
10. O. P. Agarwal, Organic Chemistry Natural Products- Vol-I and Vol- II, Geol Publishing House, 2008 and 2009.
11. M. Ramesh P S Mohan and P Shanmugam, Tetrahedron Vol. 40, p.3431 (1984).
12. M. Ramesh, P.S. Mohan and P Shanmugam, Tetrahedron Vol. 40, p.4041 (1984).
13. P.R.Iyer, S.R.Iyer and K.J. Rajendra Prasad, Indian Journal of Chemistry Vol. 23 B, p.535 (1984).
14. P.Sowmithran and K.J.Rajendra Prasad, Synthesis, 5, 545 (1985).

PAPER – III : 4. SOLID STATE CHEMISTRY

UNIT-1

The crystal systems – lattices and crystal structures – symmetry properties – crystal classes – space groups – experimental methods of X-ray diffraction for powder and single crystal samples – structural analysis and refinement – electron and neutron diffraction in the determination of structures.

UNIT II

Crystallography: Preparation of materials – crystal growth and purification, the crystal systems – lattices and crystal structures –symmetry properties – crystal classes – space groups – X – Rays – crystallography – the powder method – rotating crystal method – crystal structure determination – the structure factor – fourier synthesis of a crystal structure. Electron and neutron diffraction and structure determination.

UNIT III

The Solid State: Types of solids – close packing of spheres – binding in crystals – the bond model – the bond model – non stoichiometry – defects in solids – imperfection and physical properties – electrical, optical, magnetic, thermal and mechanical properties – magnetic materials – mixed oxides – spinels – insulators – semiconductors and super conductors.

UNIT IV

Low temperature solution growth- solution, solubility and super solubility – expression of super saturation – methods of crystallization – by slow cooling of solutions – by solvent evaporation – temperature gradient method. crystal growth system – constant temperature bath – crystallizer – filtration assembly – seed, seed mount platform and crystal revolution – unit – gel growth – introduction – principle of gel growth – various types of gel – structure of gel – growth of crystals in gels – importance of gel technique – experimental procedure – single diffusion method – double diffusion method – chemical reduction method – solubility reduction method – growth from the melt – Bridgman technique – Czochralski technique – zone refining.

UNIT V

Phase transitions – definition – Burger's classification – thermodynamic classification – Landau theory of phase transition – first order and second order transitions – structural changes with increasing temperature and pressure – martensitic transformations – order – disorder transitions. Thermal analysis – basic Principles – instrumentation – applications of thermogravimetry – differential thermal analysis and differential scanning calorimetry.

REFERENCES:

1. Physical Chemistry – W J Moore (1962).
2. Introduction to solids – L V Azarof (1960)
3. Structural Inorganic Chemistry – A F Wells, Fifth edition (1984))
4. Solid State Chemistry – N B Hannay (1976))
5 Comprehensive Inorganic Chemistry – J C Bailar et al, Vol. 4 and 5 (1975)
6. Inorganic Chemistry – Principles of Structure and Reactivity – James E Huheey 2 nd Edition (1978).

PAPER – III : 5. ORGANOMETALLIC CHEMISTRY OF TRANSITION METALS

UNIT I

Definition of organometallic compound – 18 electron rule – effective atomic number rule – 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 of metal carbonyls – the nature of M-CO bonding – binding mode of CO and IR spectra of metal carbonyls – 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 – synthesis of alkylidene complexes in low oxidation states and in high oxidation states – bonding in alkylidene complexes – synthesis and bonding in 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

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 IV

Role of organometallic chemistry in catalysis Coordinative unsaturation – oxidative addition – addition reactions of specific molecules – hydrogen addition – HX addition – addition of X2 – addition of RX – addition reactions of Si-H, C-C, C-Si and Si-Si bonds – elimination reactions - α and β eliminations – alkane activation – intramolecular and intermolecular C-H activation – activation of sulphur heterocycles – insertion of carbon monoxide – isocyanide insertion – alkene insertion – alkyne insertion.

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 ruthenium complexes in 2001 Nobel Prize for 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 1, complexes with transition metal-carbon σ-bonds, M.Bockmann, Oxford science publications, Oxford, 1996.
2. Organometallics 2, complexes with transition metal-carbon π-bonds, M.Bockmann, Oxford science publications, Oxford, 1996.
3. Basic organometallic chemistry, I. Haiduc and J. J. Zuckerman, Walter de Gruyter, Brelin, 1985.
4. Inorganic chemistry – Principles of structure and reactivity, J. E. Huheey, Harpe International Edition, Harper and Rone, New York, 1978.
5. Inorganic chemistry – Principles of structure and reactivity, J. E. Huheey, E.A.Keiter and R.L.

Keiter, Addison-Wesley Publishing Company,New York, 2000
6. Advanced Inorganic Chemistry, Sixth Edition, F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, John Wiley and sons, Inc, New York, 1999.

PAPER- III: 6. PHOTOCHEMISTRY - PHOTOPHYSICAL STUDIES

UNIT I

Some Current Topics in Photochemistry: Origin of life- mutagenic effect of radiation- photodynamic therapy– photosynthesisphotoelectrochemistry of excited state redox reations- solar energy conversion and storage.

UNIT II

Photophysical Process in Electronically Excited Molecules: Types of photophysical path ways- radiationless transition- internal conversion and intersystem crossing- fluorescence emission- fluorescence and structure- delayed fluorescence.

UNIT III

Photochemistry in Microheterogeneous Systems: General features of surfactant and lipid- excited state processes and reactions: medium effect- acid-base equilibrium in excited state- depolarization of fluorescence- excited state quenching- excimers and exciplexes- excitation energy transfer- photodimerization and photoredox reactions- structural and dynamic aspects of micellar aggregates.

UNIT IV

Photoprocesses in Molecular Inclusion Complexes: Introduction- photoprocesses in cyclodextrins- general features of cyclodextrins and inclusion complexes- fluorescence probe analysis- fluorescence depolarization- excimers and exciplex dynamics.

UNIT V

Photoprocesses in Aluminosilicates – Zeolites: General features of zeolites and their cavities- photochemistry of inorganic ions exchanged into zeolites- photochemistry of organic molecules.

References:

1. G.H. Wald, “Life and light”, Scientific American, 201, 1959, 92.
2. A. McLaren and D. Shugar, “Photochemistry of Nucleic Acid and Proteins”, Oxford, Pergamon press, 1964.
3. R.F. Reinisch, (ed.), “Photochemistry of Macromolecules”, New York, plenum press, 1970.
4. E.I. Robinowitch and Govindjee, “Photosynthesis”, New york, Wiley, 1969.
5. G. Stein, “Chemical Storage of Solar Energy and Photochemical Fuel formation”, Israel J. Chem. 14, 1975, 213.
6. K.K. Rohatgi-Mukherjee, “Fundamentals of photochemistry”, New Delhi, New Age international Publishers, 2002 (Revised edition).
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8. J.B. Birks, “Photophysics of Aromatic Molecules”, New York, Wiley, 1970.
9. J.R. Lakowicz, “Principles of Fluorescence Spectroscopy”, New York, Plenum press, 1984.

10. K. Kalyanasundaram, "Photochemistry in Microheterogeneous Systems", New York, Academic press, 1987.
11. M.L. Bender and M. Komiyama, "Cyclodextrin Chemistry", React. Struct. Concepts, Org. Chem., Vol. 16, Berlin and New York, Springer-Verlag, 1978.
12. J. Szejtli, "Cyclodextrins and their Inclusion Complexes", Budapest, Académiai Kaidò, 1982.
13. D.W. Breck, "Zeolite Molecular Sieves", New York, Wiley, 1974.
14. J.A. Rabo, (ed.), "Zeolite Chemistry and Catalysis", Acs Monograph Series, No. 171, Am. Chem. Soc., Washington, D.C. 1976.

PAPER- III : 7. PHYSICAL ORGANIC CHEMISTRY

UNIT I

1.1. Theories of Reaction Rates: Absolute reaction rate theory – thermodynamic treatment of ARRT – Significance of reaction co-ordinate – application of ARRT to simple unimolecular and bimolecular process – potential energy surfaces – partition functions and activated complexes. Eyring equation – estimation of free energy enthalpy and entropy of activation and their significance – kinetic isotopic effect 1.2. Reaction Mechanisms Principle of microscopic reversibility – steady state approximation applications.

UNIT II

2**.1 Reaction in solution Introduction** – application of ARRT to solution kinetics – the influence of solvent – the ionization of neutral molecules kinetics of ionization – reaction between ions – reaction between ions & molecules – influence of ionic – strength – primary salt effect – secondary salt effect.

2.2 Homogenous catalysis Acid-base catalysis – Hammet's acidity function Bronsted relationship – enzyme catalysis – mechanism of single substrate reactions – Michalis -Menten law- influence of pH and temperature.

UNIT III

Quantitative structure and Reactivity Relationships The linear free energy principle – (LFER) linear relationship involving difference reaction – the cettler correlation. The Hammett equation – steric effects – resonance interaction – normal substitutent constants - σ - , σ + constants – inadequancy of dual hypothesis – regularities in the through resonance effect- the Yukawa Tsuno equation – systematic deviation- steric inhabitation of resonance – Taft equation – correlation of aliphatic and aromatic relativities.

UNIT IV

Photochemistry LAWS OF PHOTO CHEMISTRY- quantum efficiency and its experimental determination – deviation and reasons- excited states and ground state, singlet and triplet states – forbidden transmissions (spin forbidden and symmetry forbidden transition) types of excitation properties of excited states – photolytic cleavage – the fate of excited molecules – physical process – Jablonski – diagram chemical processes – various types. chemiluminescence, bioluminescence, lasers, practical lasers – uses of lasers.

UNIT V

Oxidations with chromium and manganese compounds – oxidations with peracids and other peroxides – oxidation with periodic acid, lead tetra acetate, mercuric acetate - selenium dioxide. Catalytic hydrogenation and dehydrogenation metal hydride reductions and related reactions dissolving metal reductions and related reactions -reductions and the hydroactive and its derivatives.

Recommended Text Books

1. K.J. Laidler chemical kinetics, 2nd Ed. Tata Mc.Graw Hill 1975 (Unit I, II, IV)
2. W.J. Moore, Physical chemistry 5th Ed. Orient Longman 1982 (Unit I & II).
3. S. Glasstone, Text Book of Physical chemistry Mc Millan (Unit I & II).
4. Harish & Gurdeep. Advanced Physical chemistry, Goel publishing Home, Meerut (Unit I, II & IV).
5. Louis P. Hammett, Physical organic chemistry, Mc.Graw Hill Ltd., Tokyo (Unit III).
6. K.K. Rastoghi & Mukherjee, Fundamentals of Photo Chemistry, Wiley Eastern (1978) (Unit IV).
7. Advanced organic chemistry. Reactions and Mechanism's and structure – Jerry March
8. Organic synthesis – R.O.C. Normal.

References:

1. S.W. Benson, "The Foundation of Chemical Kinetics" Mc. Graw Hill, 1960.
2. C.M. Banford and E.F.M. Toiper comprehensive chemical kinetic Vol. I & I Elsevier, 1969.
3. Amdur and Hammes Chemical Kinetics – Mc. Graw Hill.
4. N.H. Turro, Molecular Photochemistry, W.A. Benjamin Reading 1965.
5. R.W. Rft. And I.C. Lowis Tetrahedron 5, 210, 1959.

PAPER- III: 8. ELECTROCHEMISTRY

UNIT I

Introduction and Principles Definition – cost of corrosion – importance of corrosion studies – classification of corrosion – expressions for corrosion rate. electrochemical principles of corrosion: Faraday's laws – types of electro chemical cells formed in corrosion process. Thermodynamic principles of corrosion: electrochemical series/ standard electrode potentials and thermodynamic corrosion theory – Galvanic series of metals and alloys and limitations. Forms of corrosion (Definition – cause and effects) : galvanic – crevice – pitting – intergranular - selective leaching – erosion - stress – hydrogen damage.

UNIT II

Kinetics of Corrosion Importance – graphical presentation of kinetic data - exchange current density – different types of polarization of electrodes. activation polarization and Tafel plots – mixed potential theory – application of electrode kinetics to experimental observations – faradic impedance and corrosion.

UNIT III

Kinetics of Passivity Introduction – electrochemical behaviour of active/passive metals – Flade potentials – criteria for selecting a metal exhibiting passivity – effects of various factors on electrochemical behaviour and corrosion rate of metal exhibiting passivity – measured versus theoretical anodic polarization behaviour – theories of passivity.

UNIT IV

Monitoring of Corrosion Determination of corrosion and corrosion inhibition parameters – non-electrochemical methods: Coupon – electrical resistance – gasometric methods. electrochemical methods: polarisation – galvanostatic – potentiostatic– potentiodynamic – AC impedance – hydrogen permeation.

UNIT V

Corrosion Control Metals and alloys – metal purification – non metallic – cathodic and anodic protection – comparison. Alteration of environment: changing the medium – use of inhibitors - classification of inhibitors – mechanism of inhibition – coating (Elementary ideas only).

References:

1. An introduction to metallic corrosion and its prevention by Raj Narayan, Oxford and IBH Publishing C., New Delhi (1983).
2. Corrosion and Corrosion control (An introduction to corrosion science and engineering) by Herbert H. Uhlig and R.Winston Review, Third Edition, A Wiley – Interscience Publication. New York (1984).
3. Corrosion engineering by Mars G. Fontana, Third Edition, McGraw Hill Book Company, Singapore (1984).
4. Application of inhibitors for acid media by G. Schmitt, Br.Corros. J., 1984. Vol.19, No.4, P.165-172.
5. Test methods for corrosion inhibitors by A.D. Mercer, Br.Corros J., 1985, Vol.20, No.2, P.61-70.
6. Inhibitors – An old remedy for a new challenge (1991 – Whitney Award Lecture) by G. Trabanelli, Corrosion, June 1991. P.410-418.

PAPER – III : 9. CHEMISTRY OF ADVANCED MATERIALS

UNIT – I

General methods of preparation, properties and applications of the following advanced materials: Liquid crystals , Ceramics (Oxide, carbides and nitrides), Thin films, Dendrimers, Zeolites, Porous membranes (anodic alumina and polycarbonate) - nanocomposites.

UNIT – II

Nanomaterials: Definition, Background- Nature and nanotechnology – Classification -0D, 1D, 2D and 3D. Types of nanomaterials – nanoparticles, nanorods, nanowhiskers – nanotubes – nanofibers. Synthesis of nanomaterials – Top-down and Bottom-up approaches – Template based synthesis – sol gel method– Physical methods - Physical vapour deposition (Evaporation and sputtering) – Chemical methods – metallorganic chemical vapour deposition (MOCVD) - Thermal decomposition – sonochemical method - chemical reduction (using sodium borohydride, hydrazine and alkali metal solutions) – photochemical reduction –biosynthesis of noble metal nanoparticles..

UNIT – III

Characterization methods in nanoscience and nanotechnology: Fundamental principles and working of the following techniques: Scanning electron microscopy (SEM) – Atomic force microscopy (AFM) – transmission electron microscopy (TEM) including high resolution transmission

electron microscopy and selected area electron diffraction pattern (HRTEM & SAED) – scanning probe microscopy (SPM) – scanning tunneling microscopy (STM) - X-ray photoelectron spectroscopy (XPS)– Energy dispersive X-ray analysis (EDAX) – X-ray diffraction (XRD) –surface plasmon resonance – surface enhanced Raman spectroscopy.

UNIT – IV

Carbon nanotubes : Structure –single walled carbon nanotubes (SWCNT)- multiwalled carbon nanotubes (MWCNT)– synthesis – solid carbon source based techniques (laser ablation and electric arc methods) - gaseous carbon based techniques (heterogeneous and homogeneous processes) - mechanism of growth of CNT - catalyst free growth and catalytically activated growth using transition metal catalysts (Root based and tip based) - Properties of CNT: Adsorption properties – transport properties – mechanical propertieschemical reactivity- Functionalisation of CNT (oxidation of CNT, reactions of oxidized CNT).

UNIT – V

Applications of Nanomaterials: Nanoelectro mechanical systems (NEMS)- Data storage devices – diskettes and tapes. Applications of CNT in catalyst support – gas storage –biosensors – CNT – metal nanocomposites – CNT – polymer composites. Biological applications of nanomaterials – Drug delivery – nanodevices in medicine. Gold nanoparticles in medicine. Catalysis using nanomaterials – metal oxide/metal nanoparticles for heterogeneous catalysis. Nanofibers for biomedical applications as an implant material. Nanomaterials for environmental applications.

References:

1. Jackie Ying - Nanostructured Materials.
2. G. Timp – Nanotechnology.
3. Robert A. Freitas Jr.- Nanomedicine, Volume I: Basic Capabilities
4. Geoffrey A. Ozin and Andre C. Arsenault, Nanochemistry – A chemical Approach to Nanomaterials, Cambridge.
5. Guozhong Cao – Nanostructures and Nanomaterials: Synthesis, Properties and Applications – Imperial College Press (2004).
6. Douglas Mulhall – Our Molecular Future: How Nanotechnology, Robotics, Genetics and Artificial Intelligence Will Transform Our World.
7. K. Eric Drexler – Nanosystems: Molecular Machinery, Manufacturing and Computation-John Wiley & Sons, Inc.: New York.
8. Reich, S., Thomsen, C. Maultzsch, J., Carbon nanotubes: Basic concepts and Physical properties, Weinheim: Wiley-VCH, 2004.
9. Nalwa, Hari Singh - Nanostructured Materials and Nanotechnology: Concise Edition, Diego: Academic Press, 2002.
10. J.Storrs Hall, Nanofuture: What's Next For Nanotechnology.
11. Norio Taniguchi – Nanotechnology : Oxford University Press.
12. Bharat Bhushan - Springer Hand Book of Nanotechnology.
13. Brown, Hemay and Bursten – Chemistry-The Central Science (6th Edition) - Published by Prentice – Hall.
14. Jose Rodriguez, Synthesis, properties and applications of oxide Nanomaterials: Wiley.
15. John Hutchison, Nanocharacterization: Royal Society of Chemistry.

PAPER- III : 10. ORGANIC SYNTHETIC METHODOLOGY AND CONFORMATIONAL ANALYSIS

UNIT I

Synthons and synthetic equivalents

Synthon approach- electron donor (nuecleophiles)-electron acceptors (electrophiles)- Chiron-umpolung-synthetic equivalents-regioselective and stereoselective alkylation of cyclic ketones, cyclic enones-selective alkylation(mono and di) via enamine reactions.

Functional group interconversions

Modern methods of functional group interconversions involving >C=O, -CHO, -OH, - SH, -COOH, >C=C<, NH_2, -COOR, CONHR functions-reversible protection of reactive sites.

UNIT II

Retrosynthetic Analysis of Simple Organic Compounds

Retrosynthetic analysis of mono & difunctional open chain target molecules and monocyclic target molecules.

Selective reactions and Reagents

Olefination of carbonyl compounds-McMurray's methods-reductions with LiAlH4 and NaBH4-Mannich reaction-Strecker synthesis-Wolf-Kishner reduction and Grignard reaction.

UNIT III

Stereochemistry and Conformational Analysis

Stereoselctive, stereospecific and regiospecific reactions- stereoselectivity in carbonyl addition-Cram's rule- configuration-conformation-torsional strain-Vander Waals strain-gauche interaction-allylic strain- conformational analysis of acylic molecules.

UNIT IV

Conformational Analysis of cyclic compounds

Conformational analysis of mono and disubstituted cyclohexanes-stability and reactivity-decalins-use of UV,IR & NMR spectroscopy for the conformational analysis of acylic and cyclic molecules-stereodynamics of fluxional moleculesvariable temperature NMR spectra (eg. N,N-dimethylacetamide)

UNIT V

Problem Solving

Solving the structure of simple organic molecules on the basis of UV,IR, NMR & Mass spectral data

References :

1. R.K. Mackie and D.M. Smith, "Guide book to Organic Synthesis", ELB, 1982.
2. Jerry March, "Advanced Organic Chemistry: Reaction and Structure" 5th Ed., Wiley 1996.
3. Silverstein and Webster, "Spectrometric Identification of Organic Compounds", 6th Ed., Wiley 1998.
4. W. Kemp, NMR in Chemistry- A Multinuclear Introduction," McMillan, 1986.
5. C.D. Becker, "High Resolution NMR- "Theory and Applications" Academic Press, 2 nd Ed., 1980.
6. R.E. Ireland, "Organic Synthesis", Prentice Hall.
7. Eliel, Stereochemistry of carbon compounds.
8. Nasipuri, Stereochemistry of organic compounds. 9. Norman, Principles of Organic Synthesis.
10. Caruthers, Some modern methods of Organic synthesis
11. Waren, Designing Organic Synthesis. A programmed introduction to synthetic approach.