

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

**(From October 2011 batch onwards)**

**PART I: PAPER – I: RESEARCH METHODOLOGY**

**PAPER – II: PHYSICAL METHODS IN CHEMISTRY**

**PAPER – III: SPECIAL PAPERS**

1. Organic Chemistry
2. Solid State and Hydrazine Chemistry
3. Organometallic Chemistry of Transition Metals
4. Chemistry of Advanced Materials
5. Photochemistry of – Photophysical Studies
6. Environmental Chemistry
7. Chemistry of Crystalline Solids
8. Physical Organic Chemistry
9. Electro Chemistry
10. Polymer Chemistry
11. 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**

#### **Dissertations:**

Nature and purpose, components and preparation, Writing techniques- introduction, word processing and layout, writing and formatting with the computer, Figures-general considerations, line art, drawing with a computer and half tones. Tables-logic, significance, form, components, worksheets, list and database.

#### **Collection and Citation of Literature:**

Acquisition of information, building up of own literature collection, citation techniques, forms of citation, anatomy of source description.

#### **Publication of Journal Articles:**

Concept, electronic publication, types of journals, 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 in chemical analysis – classification of errors – determination of accuracy of methods –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**

#### **Flame emission and atomic absorption**

#### **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 – Applications of atomic emission spectroscopy – flames and flame spectra.

#### **Fluorometric analysis:**

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 spectroscopy.

#### **HPLC:**

Principles of high performance liquid chromatography – the liquid chromatograph – the requirements of solvent pumping and different pumping systems – gradient elution, isocratic elution, sampling – detectors for liquid chromatography – the mobile phase in HPLC – solvent degassing – column technology – column selection – quantitative analysis by HPLC.

**UNIT - V****Electroanalytical methods :**

redox potentials – definition – Methods of determination – applications – ion selective electrodes. Current – voltage relationships – polarography – instrumentation – characteristics of DME – diffusion current – half wave potentials. Amperometric titrations - constant 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. Russcy , WILEY-VCH Verlas Gmbh & Co, K G a A.Wecnhcim 2<sup>nd</sup> Edn(2004)
2. Spectrometric identification of organic compounds – R.M.Silverstein, G.C. Bassler and Morrill. John Wiley & Sons, New York 5<sup>th</sup> Edn (1991).
3. Physical methods in Inorganic chemistry – R.S.Drago . Recnhold Pub.Corp.,(1965)
4. Physical methods in Organic Chemistry – Scharz. Oliver & Boxd,(1964)
5. Applications of absorption spectroscopy of organic compounds – J.Dyer.
6. Organic spectroscopy – W.Kemp. Macmillan, (1987)
7. An introduction to spectrometric methods for the identification of organic compounds Vol.I& II – F.Schlenmann. Pergamon Press, oxford (1970)
8. Introduction to spectroscopy – A guide for students of organic chemistry – D.L.Pavia,G.M.Lampman and G.S.Kniz Jr.
9. Instrumental methods of analysis – H.Willard, L.Merrit Jr.and A.Dean. 4<sup>th</sup> Edn(1996)
10. Principles of instrumental analysis –D.A.Skoog and M.West. 2<sup>nd</sup> Edn, Saunders College,(1980)
11. Instrumental methods of chemical analysis – B.K.Sharma. Krishna Prakashan
12. Fundamentals of analytical chemistry – D.A.Skoog and M.West.7<sup>th</sup> Edu, Saunders College Pub (1996)
13. Analytical chemistry – J.D.Dick. American Chemical Society (2007)
14. Basic concepts of analytical chemistry – S.M.Khopkar. Wiley(1984)
15. Fundamentals of molecular spectroscopy – C.N.Banwell. 4<sup>th</sup> MC. Graw- Hill,(2008)
16. Basic principles of spectroscopy – R.Chang.
17. Spectroscopy of organic compounds – P.S Kalsi. New Age International 6<sup>th</sup> Edn (2009)

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**M.Phil / Ph.D CHEMISTRY**

**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 Molecularstructure–chromophoricgroups –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 or common functional groups – applications.

**UNIT II**

**<sup>1</sup>H and <sup>13</sup>C NMR Spectroscopy:**

Proton chemical shifts – aromatic ring systems – anisotropic effects – <sup>13</sup>Carbon chemical shifts – mechanisms 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 <sup>13</sup>C spectrum – INDOR and nuclear overhauser effect (NOE) – <sup>13</sup>C relaxation mechanisms – measurement of <sup>13</sup>C- relaxation times- Spin- lattice relaxation (T<sub>1</sub>) and pin – spin relation (T<sub>2</sub>) measurements – assignment <sup>13</sup>C technique in <sup>13</sup>C spectra – 2D-NMR –COSY, HETCOR, NOESY, ROESY-DEPT. <sup>13</sup>C. SPECTRA-INADEQUATE, spectrachemical shift correlation –quantitative measurement in <sup>13</sup>C – NMR – relaxation reagents – intensity standards.

**UNIT IV**

**ESR Spectroscopy:**

Theory – instrumentation – derivative curves ‘g’ values – ‘g’ shift – origin of hyperfine splitting –isotropic systems – anisotropic systems – anisotropic effect zerofield splitting – Kramer’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 molecular weights and formulae – metastable peaks – nitrogen rule – ion fragmentation mechanisms – rearrangements – use of mass spectrometry in the structural elucidation of organic compounds – mass spectra of compounds containing different functional groups.

### REFERENCES:

1. Proton and Carbon -13 NMR Spectroscopy – An Integrated Approach – R.J.Abraham and Loftus.
2. Spectroscopy of organic compounds, P.S.Kalsi, new age international publisher (2002)
2. Spectroscopic Identification of Organic Compounds – R.M.Silverstein, G.C.Bassler and Morrill.
3. Physical Methods in Inorganic Chemistry – R.S.Drago.
4. Physical Methods in Organic Chemistry – Scharz.
5. Applications of NMR Spectroscopy in Organic Chemistry – Jockmann and Strenhell.
6. Applications of absorption spectroscopy of organic compounds – J.Dyer.
7. Interpretation of Mass Spectra – McLafferty.
8. Interpretation of Mass Spectra of Organic Compounds – Budzikowiex, Djerassi and Williams.
9. NMR of Organic Chemists – Mathioson
10. Electron Spin Resonance – Elementary Theory and Practical Applications – Wertz and Bolton
11. Mass Spectrometry for Organic Chemistry – Raw Johnstone.
12. Interpretation of NMR Spectroscopy –R.H.Bible.
13. High Resolution NMR - Becker.
14. Interpretation of Mass Spectra of Organic Compounds – Hamming and Foster.
15. Interpretation of  $^{13}\text{C}$  NMR - F.W.Wehrli, T.Wirthlin and Heydon.

## PAPER-III 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 Oxides.
- 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 photochemical 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 Depletion – 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 pyrolysis – 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 Limited, New Delhi, Second Edition,1987.



**BHARATHIAR UNIVERSITY::COIMBATORE – 46****M.Phil / Ph.D CHEMISTRY****PAPER – III: 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  $\alpha$ -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' Cornell 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).
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- 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.