BHARATHIAR UNIVERSITY : COIMBATORE-640 046.

M.Phil./Ph.D. – CHEMISTRY

for the year 2009-2010 and onwards

PART – I SYLLABUS

PAPER – I - Research Methodology

PAPER- II - Physical Methods in Chemistry

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PAPER – I : RESEARCH METHODOLOGY

UNIT I

Data Analysis:

Errors in chemical analysis – classification of errors – determination of accuracy of methods – improving accuracy of analysis – significant figures – mean, standard deviation – cpmparison 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 II

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 III

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 IV

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.

UNIT V

Mossbauer Spectroscopy:

Introduction – resonance like shifts from change in electron environment – quadrupole interactions – magnetic Interactions - applications.

Nuclear Quadrupole Resonance Spectroscopy:

Introduction – effect of a magnetic field on the spectra – relationships between the electric field gradient and molecular structure – applications – the interpretation of eQq data – the effects of crystal lattice on the magnitude of eQq – structural information from NQR spectra.

REFERENCES:

1. Spectrometric identification of organic compounds – R.M.Silverstein, G.C. Bassler and Morril.
2. Physical methods in Inorganic chemistry – R.S.Drago.
3. Physical methods in Organic Chemistry – Scharz.
4. Applications of absorption spectroscopy of organic compounds – J.Dyer.
5. Organic spectroscopy – W.Kemp.
6. An introduction to spectrometric methods for the identification of organic compounds Vol.I & II –F.Schienmann.
7. Introduction to spectroscopy – A guide for students of organic chemistry – D.L.Pavia, G.M.Lampman and G.S.Kniz Jr.
8. Instrumental methods of analysis – H.Willard, L.Merrit Jr.and A.Dean.
9. Principles of instrumental analysis – D.A.Skoog and M.West.
10. Instrumental methods of chemical analysis – B.K.Sharma.
11. Fundamentals of analytical chemistry – D.A. Skoog and M.West.
12. Analytical chemistry – J.D.Dick.
13. Basic concepts of analytical chemistry – S.M.Khopkar.
14. Fundamentals of molecular spectroscopy – C.N.Banwell.
15. Basic principals of spectroscopy – R.Chang.

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PAPER-II : PHYSICAL METHODS IN CHEMISTRY

UNIT I

U.V.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.

I.R. Spectroscopy:

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

UNIT II

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

Porton chemical shifts – aromatic ring systems – anisotropic effects – ^{13} Carbon chemical shifts – mechanisms of spin-spin coupling – vicinal, geminal 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) – ^{13}C relaxation mechanisms – measurement of ^{13}C relaxation times – spin – lattice relaxation (T_1) and spin – spin relation (T_2) measurements –assignment technique in ^{13}C spectra – chemical shift correlation – quantitative measurement in ^{13}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 – 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 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. Spectroscopic Identification of Organic Compounds – R.M.Silverstein, G.C.Bassler and Morril.
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 – Budcikowiex, 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}C NMR Spectra – F.W.Wehrli, T.Wirthlin and Heydon.
