

SYLLABUS

(For candidates admitted from 2009 – 2010)

MCH1 RESEARCH METHODOLOGY

UNIT – I

Research methods – Identification of the Problem – Determining the mode of attack -Literature survey – Mode of approach of actual investigation – Abstraction of a research paper – Drawing inferences from data - Qualitative and Quantitative analysis – Internet and its applications – e-journals- Assessing the status of the problem – Results and Conclusions – Presenting a Scientific seminar – Publication of Research paper - Art of writing a Thesis.

UNIT – II

Survey of literature including patents - chemical nomenclature and literature primary sources - secondary sources including reviews. Treatise and monographs, literature searching, Review of work relevant to the chosen problems.

UNIT – III

Writing a thesis or paper - General formation - page and chapter formation. The use of quotation - footnotes - tables and figures - referencing - appendixes - revising the paper or thesis - editing and evaluating and the final product - proof reading - the final types copy.

UNIT – IV

Iterative methods: Newton Raphson iterative method – Secant Method; Interpolation: Newton's forward and backward difference formulae; Differentiation and Integration: Numerical differentiation with interpolation polynomials – Numerical Integration by Trapezoidal and Simpson's rule- Ramberg integration.

UNIT – V

Introduction – C++ fundamentals – Structure of C++ Program – Control Statements – Arrays – Functions – Character handling in C++ - Pointers – Structure and Unions – Classes and Objects – Inheritance – Input and Output Operations in C++ - Advanced Features in C++ - Simple Programs in C++.

Reference Books

1. Thesis and Assignment Writing – J Anderson, B.H. Dursten and M. Poole, Wiley Eastern (1977).
2. Research Methodology (Second Revised Edition) – C.R.Kothari; New Age Publishers, 2004 (Chapters 1 – 11).
3. Computer Oriented Numerical Methods – V. Rajaraman, Prentice Hall of India.
4. Numerical Methods for Scientific and Engineering Computation – MK Jain, SRK Iyengar and RK Jain, Wiley Eastern publ.
5. Programming with C++ - P. Radha Ganesan SCITECH, 2002.
6. Programming with C++ - D. Ravichandran TATA McGraw Hill, 2001.

MCH2 PHYSICAL METHODS IN CHEMISTRY

UNIT-I:

UV-Visible Spectroscopy: Electronic transition-chromophores and auxochromes-factors influencing position and intensity of absorption bands-absorption spectra of dienes,polyene and unsaturated carbonyl compounds-woodward Fieser rules –effect of solvent on spectra.

IR Spectroscopy: Vibrational frequencies and factors affecting them-identification of functional groups – intra and inter molecular hydrogen bonding –finger print region-far IR region.

UNIT-II

H¹ NMR Spectroscopy: H¹-NMR chemical shift – chemical and magnetic equivalent –homotopic, enantiotopic diastereotopic relationships – coupling constants germinal and vicinal and long range coupling constants-criteria for first order and non first order spectra factors influencing proton chemical shift and vicinal proton – proton coupling constants Karplus equation. H¹-NMR spectra of some organic and inorganic molecules –spin decoupling –nuclear Overhauser effect-chemical exchange.

C¹³ NMR Spectroscopy: Introduction - Proton decoupled and off resonance C¹³ NMR Spectra-factors affecting C¹³ chemical shifts -C¹³ NMR Spectra of some organic molecules.

UNIT-III

EPR Spectroscopy: Factors affecting the magnitudes of g and A tensors in metal species –zero field splitting and Kramers degeneracy-spectra of V(II), Mn(II), Fe(II), Co(II), Ni(II) and Cu(II) complexes-Application of EPR to a few biological molecules containing Cu(II), Fe(II) and Fe(III) ions –densities and McConnell relationship-application of EPR to some simple system such as CH₃, p-benzoquinone and Xe²⁺.

Mossbauer Spectroscopy: Isomer shifts-magnetic interactions- Mossbauer emission spectroscopy-applications to iron and tin compounds.

UNIT- IV

Mass Spectroscopy: Principles and measurement techniques(EI,CI,FD,FAB,SIMS)-Presentation of spectral data –molecular ions –isotope ions –fragment ions of odd and even electron types –rearrangements of ions –factors affecting cleavage patterns –general fragmentation patterns-Mc Lafferty rearrangement –Retro Diels –Alder fragmentation.

ORD & CD: Principles – circular birefringence and dichroism-cotton effect –ORD curves –application on cotton effect curves -α-Haloketone rule-octant rule-applications for determination of conformation and configuration.

UNIT - V

Electro analytical techniques: Principle and applications of electrogravimetry-coulometric analysis-Dcpolarigraphy-Cyclic Voltametry-stripping analysis.

Spectroanalytical Techniques: Principles and application - Atomic absorption spectroscopy, atomic emission spectroscopy – photo electron spectroscopy.

Reference Books:

1. Dyer.J.,R, Applications of absorption spectroscopy of organic compounds, Prentice - Hall, 1978.
2. Silverstein and Webster, Spectrometric Identification of Organic Compounds, Sixth Edition Wiley, 1998.
3. Kemp.W., Organic Spectroscopy, 3rd Edition, ELBS, New Delhi, 1989.
4. Lambert. J.B, Shurrell. H.F., Lightner. AP., and Cooks.R.G., Introduction to Organic Spectroscopy, Macmillan, 1987.
5. Stothers,J.B., Carbon-13 NMR Spectroscopy, Academic press, 1972.
6. Drago. RS., Physical Methods in Chemistry, W.B. Saunders Company, London, 1999.
7. Drago, RS., Physical Methods in Inorganic Chemistry, 3rd edition, Wiley Eastern Company.
8. Kalsi, P.S., Organic Spectroscopy, Tata McGraw Hill, New Delhi.
9. Willard, H.H., Merritt,L.L., and Dean JA, Instrumental Methods of Analysis, East-West Press, New Delhi, 1988.