

NATIONAL COLLEGE (AUTONOMOUS) TIRUCHIRAPALLI-620 001.
M.PHIL CHEMISTRY

(For the academic admitted from the academic year 2013-2016 onwards)
CORE COURSE I: PHYSICAL METHODS IN CHEMISTRY

UNIT-I

Electronic Absorption Spectroscopy

Principles of Absorption Spectroscopy – Chromophore – UV – Visible Spectroscopy – Application to organic compounds – Woodward – Fieser and Scott rules for conjugated dienes and polymers – Ketones, Aldehydes, α,β -unsaturated acids, Esters, Nitriles and amides. Woodward's rule for enones- differentiation of geometrical isomers and positional Isomers- Di substituted Benzene derivatives- study of steric effect on aromaticity .

Microstates – Term symbols and energy level for d^1 – d^9 ions in cubic and square fields – Intensity of bands-group theoretical approach to selection rules- effect of distortion and spin – orbit coupling on spectra- Evaluation of $10Dq$ and β values for octahedral complexes of cobalt - applications to simple coordination compounds- charge transfer spectra.

UNIT-II

Infra red spectroscopy

Vibration in simple molecules (H_2O , CO_2) and their symmetry notation for molecular vibration – group vibration and the limitations – combined uses of IR and Raman Spectroscopy in the structural elucidation of simple molecules like N_2O , ClF_3 , NO_3^- , ClO_4^- - effect of coordination on ligand vibration – uses of group vibrations in the structural elucidation of metal complexes of thiourea, cyanide, thiocyanate, nitrate, sulphate and Dimethyl sulphoxide – effect of isotopic substitution the vibrational spectra of molecules- Vibrational spectra of metal carbonyls with reference to the nature of bonding, geometry and number of C-O stretching vibration (group theoretical treatment)

The modes of stretching and bending – FT-IR sampling techniques- correlation tables – for functional groups - alkanes, alkenes, alkynes, aromatic rings, alcohols, carbonyl compounds- factors that influence $>C=O$ stretching vibration – hydrogen bonding (inter, intramolecular).

UNIT-III

Nuclear magnetic Resonance spectroscopy

1H NMR long – range coupling – Homotopic, enantiotopic and diastereotopic systems – conformationally mobile, open – chain system – virtual coupling – coupling of protons to fluorine, phosphorous – nuclear overhauser effect .

^{13}C NMR – off resonance decoupling – coupling of carbon to deuterium, fluorine, phosphorus- DEPT- applications of proton and carbon data in identifying small organic compounds.

2D NMR : principles of 2D NMR Spectroscopy - 1H - 1H COSY- 1H - ^{13}C COSY – HMBC- HSQC.

Basic principles of solid state NMR

UNIT-IV

Electron paramagnetic resonance spectroscopy

Basic concept of ESR Spectroscopy- factors affecting the magnitude of g and A tensors in metal complexes-anisotropy in g and A values – zero-field splitting and Kramers degeneracy - application of EPR to some simple inorganic systems like methyl radical, p-benzosemiquinone and naphthalene anion, Cu(II), Fe(II), Mn(II) and VO(IV) complexes- spin - trapping .

UNIT-V

Mass spectrometry and its applications

Mass spectra introduction – parent peak, base peak ,isotopic peak, metastable peak - ionization techniques – chemical ionization, field desorption fast atom – ion bombardment (FAB) – Electrospray Ionisation (ESI)- Matrix – Assisted Laser Desorption/ Ionization (MALDI)

Resolution and determination of molecular formula – mass analyzers magnetic field only. doublefocussing, quadrupole ion storage, time of flight (TOF), -hyphenated techniques – GC-MS, LC-MS and tandem mass spectrometryMS/MS

REFERENCES

UNIT-I

1. A.B.P. Lever, 'Inorganic Electronic Spectroscopy' ,American Elsevier, 1986.
2. R.S Drago, 'Physical Methods In Inorganic Chemistry', 3rd Edition Wiley Eastern company.

UNIT-II

1. R.S Drago, 'Physical methods in inorganic chemistry',. 3rd Edition Wiley Eastern company.
2. N.B. Clothup, L.H. Daly and S.E. Wiberly , 'Introduction To Infrared And Raman Spectroscopy' Academic press ,New york , 1975.
3. R.S Drago , 'physical methods in chemistry'. W.B Saunders company, Philadelphia, 1977
4. D.N Sathiyararyana, 'Vibarrational Spectroscopy' , New Age International publishers New Delhi.
5. K.Nakamoto ` Infrared spectra of Inorganic and Coordination compounds' . . 2nd edition , Wiley –inter Science ,New york.
6. D.L .Pavia, G..M Lampmann and G.S Kriz ,'Introduction to Spectroscopy' 3rd edition , Brooks Cole ,2000.

UNIT-III

- 1.P.M Silverstein and F.X. Webster, 'spectroscopic Identification of Organic Compounds' , 6th edition, John Wiley andSons, 1998.
2. J. Mohan, 'Organic Spectroscopy : Principles and Applications',CRC: 2nd edition, 2004
3. W. Kemp, 'Organic Spectroscopy', 3rd ed., Macmillan, 1994.
4. D.L.Pavia, G.M. Lampmann and G..S. Kriz, ` introduction to spectroscopy', 3rd ed., Brooks Cole, 2000.
5. H. Gunther, 'NMR spectroscopy- Basic Principles, Concepts and Applications in Chemistry', 2nd edition, John Wiley and Sons, 1995.

UNIT-IV

1. R.S. DRgo, 'Physical Methods in Inorganic Chemistry, 3rd edition, Wiley Eastren Company.
2. R.S. Drago, 'Physical Methods in Chemistry', W.B. Saunders Company, 1977.
3. J.A. Weil, J.R. Bolton and J.E. Wertz, 'Electron Paramagnetic Resonance; Elementary Theory and Practical Applications, John wiley and Sons, 1994.

UNIT-V

1. P.M. Silverstein and F.X. Webster, 'Spectroscopic Identification of Organic Compounds', 6th ed., John Wiley and Sons, 1998.
2. Theme Issue on " Frontiers in Mass spectrometry", Chem. Rev. 2001, Vol. 101. p xxx Bioanalytical Chemistry, S.K. Mikkelsen and Eduardo Corton, Wiley-Interscience-John-Wiley and sons, Inc., 2004.

CORE COURSE II: ANALYTICAL TECHNIQUES IN CHEMISTRY

UNIT I

Instrumental Methods of Analysis

Basic aspects of synchronous fluorescence spectroscopy- Phosphorescence- spectral hole burning - flow cytometry- instrumentation on fluorescence ratio- fluorimeters (quantization).

Structural methods: Extended X-ray absorption fine structure(EXAFS) - Surface extended X-ray absorption (SEXAFS). Operation modes of lasers-types of lasers-physical applications of lasers: non-linear optical effects-laser systems as remote sensors-recent advances in analytical laser spectroscopy-isotope analysis, small molecules and radicals with pulsed lasers, coherent anti-Stokes Raman spectroscopy(CARS)

UNIT-II

Chromatography and Separation Techniques

Solvent extraction -Principles of ion exchange ,paper ,thin layer and column chromatography -Gas chromatographic techniques - Columns, adsorbents, methods, R_f values ,Mc Reynold's constant and their uses- HPTLC, HPLC techniques -adsorbents columns ,detection methods - estimation -preparative column -GC-MS techniques methods ,principles and uses.

Electrophoresis :Principles ,factors affecting ionic migration -Effect of P^H and ionic strength - Gel electrophoresis.

UNIT-III Electro analytical Techniques

Linear -sweep voltammetry - cyclic voltammery -Reversibility ,elucidation of reaction mechanisms -differential pulse voltammetry - potentiometric stripping analysis -chronocoulometry - chronopotentiometry ,Electro chemical sensors ,ion- selective electrodes, glass-membrane electrodes, solid-liquid membrane electrodes- ion-sensitive field effect transistors (ISFETs) - Sensors for the analysis of gases in solution - Amperometric gas sensors.

UNIT -IV

INTRODUCTION TO GREEN CHEMISTRY AND TECHNIQUES

Green chemistry -relevance and goals, Anastas

Twelve principles of green chemistry -Tools of green chemistry : alternative starting materials, reagents, catalysis, solvents and processes with suitable examples .

Microwave mediated organic synthesis - Microwave activation - advantage of microwave exposure -specific effects of microwave -Neat reaction -solid supports reaction -Functional group transformation - condensation reactions -Oxidations -reduction reactions -multi-component reactions.

UNIT-V

MICROSCOPY TECHNIQUES

Electron Microscopy -Scanning electron microscopy (SEM)- Transmission electron microscopy(TEM) -general design ,resolution ,electron sources ,TEM grids, electron lenses, electron -sample interaction -Scanning transmission electron microscopy (STEM)

Scanning probe microscopy : atomic and molecular force microscopes (AFM and MFM) -Scanning tunneling microscope (STM) -Scanning nearfield far field optical microscope (SNOMand SFOM)-Scanning ion

conductance microscope –scanning Thermal Microscope –Fluorescence microscope.

References:

UNIT-I

1. A.Sharma, ,S.G.Schulman "Introduction to Fluorescence Spectroscopy", Wiley – Interscience, New York,1999
2. F.Rouessac and A. Rcuessac, ' Chemical Analysis', John Wiley and Sons, Chichester 2000.
3. C.N Banwell and E.M McCash ,Fundamentals of Molecular Spectroscopy '4th edition ,Tata McGraw –Hill ,New Delhi ,1994.
4. Nicolo Omemetto, 'Analytical Laser Spectroscopy ' , Vol.50 John –Wiley and sons, New York,1979.

UNIT-II

- 1.R.Stock and C.B.F.Rice, 'Chromatographic Methods' , Chapman and Hall ,New york,1963
2. B.S Furniss ,A.J.Hannaforde ,P.W.G.Smith and R.Tatchell ,"Vogel's Text book of practical Organic Chemistry" , 5th Edition, Pearson, New Delhi ,1989
3. V.K .Srinivastava and K.K .Srivastava ,' Introduction to Chromatography ' , 2nd edition, S.Chand and Co ., New Delhi ,1981.

UNIT –III

1. C.H .Hamann ,A. Hammett and W. Vilestich, 'Electrochemistry' ,Wiley VCH ,1998
2. A.J. Bard and L.F .Faulkner, ' Electrochemical methods –Fundamental and applications', 2nd edition ,Wiley –VCH ,1998
3. AC .Fisher, 'Electrode dynamics' , Oxford University Press, 1996
4. J.Koryta and K.Stulik , ' Ion-Selective Electrodes',Cambridge University press,1983
5. J.Janata, 'Principles of Chemical sensors', plenum Press,New York 1989

UNIT –V

- 1.V.K Ahluwalia, 'Green Chemistry –Environmentally benign reactions', 'Ane Books India (publishers T.Anastas) ,2006
- 2.Paul T. Anastas and Tracy C.Williamson ,'GreenChemistry –Desinging Chemistry for the Environment' , Second Edition., 1998.
3. Paul T. Anastas and Tracy C.Williamson ,'GreenChemistry –Frontiers in benign chemical synthesis and processes' , Oxford university press, 1998.
4. Rashmi Sanghi and M.M Srivastava ,'Green Chemistry –Environment friendly altenative', Narosa publishing house, 2003.

UNIT-V

1. Special Issue on Nanoscience ,Acc. Chem. Res.,41(12) December 2008
2. Bengt Nolting, ' Methods in Modern Biophysics' ,Springer ,2004.
3. T.Pradeep , Nano : The Essentials ` Tata McGraw Hill ,New Delhi, 2007
4. H.Fujita ,' Micromachines as Tools in NanoTechnology ,' Springer –Verlag , Berlin 2003.

RESEARCH METHODOLOGY

UNIT-I : Selection of Research problems and Survey of Scientific Literature

Primary source of journals and patents-secondary sources-listing of titles-abstracts-Beilstein- compendia and tables of information-reviews –general treatises-monographs and treatises on specific areas-literature searching-information about a specific compound-science citation index - Box to locate journals.

UNIT-II: Data analysis

Precision and accuracy-reliability-Determinate and random errors-distribution of random errors –normal distribution curves- statistical treatment of finite samples- T- test and F- test. Criteria for the rejection of an observation-Q-test-significant figures and computation rules- data plotting- least square analysis-significance of correlation coefficient.

UNIT III: Thesis and Paper writing

Conversions in writing-general format- page and chapter format- use of quotations and footnotes- preparation of tables and figures- references-appendices - revising editing and evaluating the final material - proof reading meanings and examples of commonly used abbreviation.

UNIT-IV: Educational technology

Origin, history, meaning and definitions of educational technology-objectives, form and approaches-scope, significance and use of educational technology-system concept-types-parameters-system approach –education system instructional system.

UNIT V: Information and Communication Technology

Meaning of information and communication technology(ICT)- definition-features – trends - uses and limitations - characteristics of e-learning-advantages and limitations - integration of ICT in teaching and learning - ICT applications: using word processors, spread sheets, power point slides in the class rooms- ICT for research: online journals, e-books, technical reports, thesis and dissertations - computer mediated teaching: multimedia e - content.
