MASTER OF PHILOSOPHY IN CHEMISTRY
SYLLABUS SESSION 2013-14

CURRICULUM

Sl. No	Code	Papers	Max. Marks	Ex. Hrs.
1	**MPCH 101**	Research Methodology	100	3
2	**MPCH 102**	Physical Methods in Chemistry	100	3
3	**MPCH 103**	Specialization on dissertation topic	100	3
4	**MPCH 104**	Dissertation	100	-

RESEARCH METHODOLOGY THEORY AND TECHNIQUES
MPCH 101

(Bio Technology, Biochemistry, Botany, Chemistry, Commerce, Computer Science, Corporate Secretaryship, Education, Education, Electronics, Information Technology, Microbiology, Home Science, Hotel Management, Hotel Management, Library Science, Management, Physics, Population Studies, Psychology, Public Administration, Sociology, Tourism Management, Zoology)

UNIT - I

Research – Definition – Importance and Meaning of research – Characteristics of research – Types of Research – Steps in research – Identification, Selection and formulation of research problem – Research questions – Research design – Formulation of HypoDissertation – Review of Literature.

UNIT – II

Sampling techniques: Sampling theory – types of sampling – Steps in sampling – Sampling and Non-sampling error – Sample size – Advantages and limitations of sampling. Collection of Data : Primary Data – Meaning – Data Collection methods – Secondary data – Meaning – Relevances, limitations and cautions.

UNIT – III

Statistics in Research – Measure of Central tendency – Dispersion – Skewness and Kurtosis in research. HypoDissertation – Fundamentals of HypoDissertation testing – Standard Error – Point and Interval estimates – Important Non-Parametric tests : Sign, Run, Kruskal – Wallis tests and Mann-Whitney test.

UNIT – IV

Para metric tests: Testing of significance – mean, Proportion, Variance and Correlation – testing for Significance of difference between means, proportions, variances and correlation co-efficient. Chi-square tests – ANOVA – One-way and Two-way

UNIT – V

Research Report: Types of reports – contents – styles of reporting – Steps in drafting reports – Editing the final draft – Evaluating the final draft.

Reference Books:

1. Statistical Methods — S.P. Gupta
2. Research Methodology Methods and Techniques — C.R. Kothari
3. Statistics (Theory and Practice) — B.N. Gupta
4. Research Methodology Methods and Statistical Techniques — Santosh Gupta

PHYSICAL METHODS IN CHEMISTRY
MPCH 102

UNIT- I

Electronic spectroscopy: Microstates – term symbols and energy levels for d1-d9 icons I 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 Beta values for octahedral complexes of cobalt and nickel - application to simple coordination compounds – charge transfer spectra.

UNIT- II

Infrared and Raman spectroscopy: Vibrations in simple molecules and their symmetry notation – group vibrations and the limitations-applications of Raman spectroscopy – combined uses of IR and Raman spectroscopy in the structural elucidation of simple molecules – effect of coordination on ligand vibration – uses of group vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocynate, nitrate, sulphate and dimethyl sulfoxide-effect of isotopic substitution on the vibrational spectra molecule – vibrational spectra of metal carbonyls with reference to the nature of bonding, geometry and number of C-O stretching vibrations – applications of Raman spectroscopy.

Sampling techniques, factors influencing group frequencies – both internal and external quantitative studies, hydrogen bonding conformational aspects in cyclic 1,2 diols and 1,3 diols, H NMR spectroscopy – coupling constant – first order and second order splitting spin-spin splitting - dependence of J on dihedral angle-vicinal and geminal coupling constants- karplus equation- long range, coupling constants, influence of stereo chemical factors on chemical shift of protons, simplification of complexes spectra-double resonance techniques, shift reagents, chemical spin decoupling of rapidly exchangeable protons(OH, SH, COOCH, NH, NH2)-an elementary treatment of NOE phenomenon-2D technique (COSY, NOESY, and rosy)- 13C NMR spectroscopy. Basic theory of FT-NMR-relaxation-broad band decoupling. Off resonance and chemical shift correlations (CH,CH2, CH3, =CH2=,aromatic)

UNIT-III

NMR Spectroscopy: principles and methods, Definition of nuclear angular momentum and the nuclear magnetic moment: idea about the rotating axis, Bloch equations, the quantum mechanical description of the NMR experiment, transition probabilities, relaxation effects, Fourier transform NMR – measurement of T1 and T2. Effect of quadrupolar nuclei evaluation of thermodynamic and kinetic data using NMR techniques, second order spectra – quantum mechanical treatment of coupling, effects of relative magnitudes of J on the spectrum of an AB molecule, double resonance experience, Spectral simplication and determination of signs of coupling constants

Examples for different spin systems – chemical shift and coupling constants involving different nuclei (1H, 19F, 31P, 13C) interpretation and applications to inorganic compound. Effects of quadrupolar nuclei (2H, 10B, 11B) on the proton NMR spectra satellite spectra.

Systems with chemical exchange – evaluation of thermodynamic parameter in simple systems – systems of fluxional behavior of molecules and elementary treatment of second order spectra – examples – NMR of paramagnetic molecules – isotropic shits contact and pseudo- contact interactions – lanthanide shift reagents – Characteristics of quadrupolar nucleus – effect of field gradient and magnetic field upon quadrupolar energy levels – NMR transitions – applications.

UNIT-IV

EPR Spectroscopy: Factors affecting the magnitude of g and A tensors in metal species –zero field splitting and Kramer's degeneracy – spectra of VO(II), Mn(II), Fe(II), Co(II), Ni(II) and Cu(II) complexes. Applications of EPR to a few biological molecules containing Cu(II), Fe(II)and Fe(III) icons-spin densities and McConnell relationship – applications of EPR to some simple system such as CH3, P-benzosemiquionon, Xe2+. Mass Spectrometry – instrumentation resolution, EI and CI methods – base peaks, metastable peak, parent peak, determination and use of molecular formula, Recognition of molecular ion peak –FAB –fragmentation – general rules – pattern of fragmentation for various classes of compounds, McLafferty rearrangement, importance of metastable peaks.

UNIT-V

Optical Rotary, Dispersion and Circular Dictorism, ORD and CD cotton effect – octant rule, alpha- haloketond rule – applications to determining absolute configuration of simple monocyclic ketenes and metal complexes

UNIT –VI

Moss Bauer Spectroscopy: Isomeric shifts – magnetic interactions – Moss Bauer emission spectroscopy – applications to iron and tin compounds.
Photo electron Spectroscopy: Principles – Auger electron spectroscopy – electron spectra in chemical analysis.

UNIT –VI

Diffraction Methods: Crystal symmetry – combination of symmetry elements – crystal classes – screw axis and glide planes – space group – crystal axes, crystal systems, unit cell, bravis lattices, asymmetric and crystallographic symmetry – basic concepts and examples, The concept of reciprocal lattice and its application s – X-ray diffraction by single crystals – structure factor – determination of space group by symmetric phase problem in structure analysis heavy atom method – Fourier synDissertation – refinement of structure
Neutron diffraction – magnetic scattering – applications and comparison with X-ray diffraction
Electron diffraction – basic principles and applications to simple molecules- XeF6, Be(BH4)2, ferrocene, Cr(II) acetate

Reference books:

1. R.S DRAGO, “Physical Method in Inorganic Chemistry”, 3rd ed., Wiley eastern company (I,II,III & IV).
2. R.S DRAGO, “Physical Methods in Chemistry”, W.B. Saunders Company, Philadelphia, London P.J. Wheately
3. “The Determination of Molecular Structure”,(V) E.A.V. Ebsworth,
4. “Structural Methods in Inorganic Chemistry”, 3rd ed., ELBS, Great Britain, 1987 B.P. Straughan and S. Walker,
5. “Spectroscopy Vol. I”, Chapman and Hall (1976). C.N. Banwell,
6. “Fundamentals of Molecular Spectroscopy”, 3rd ed., McGrawhill, 1983, New Delhi. W. Kemp,
7. “NMR in chemistry A Multinuclear Introduction”, McMillan, 1986.