COURSES OF STUDY AND SCHEME OF EXAMINATION

ACADEMIC YEAR 2014-2015 ONWARDS

SERIAL NUMBER	NAME OF THE PAPER	INTERNAL	EXTERNAL	MAX MARKS	CREDIT
1	CORE I—MPPH1 RESEARCH METHODLOGY	25	75	100	6
2	CORE I—MPPH2 ADVANCED TOPICS IN PHYSICS	25	75	100	6
3	ELECTIVE (any one) X-RAY CRYSTALLOGRAPHY-MPPHE1 CRYSTAL GROWTH-MPPHE2	25	75	100	6
4	DISSERTATION-MPPHPR	50	150	200	18
			TOTAL	500	36

CORE PAPER –I

RESEARCH METHODOLOGY - Credit-6

I : PRINCIPLES OF SCIENTIFIC RESEARCH

1. Nature of research – History of research- research and philosophy-the mental approach-the planning of research-the organization of research-experimentation-accuracy and economy of effort-social implications of research-relevance of research in modern society.
2. Use of library- use of abstracts-preparation of bibliography-methods of editing-presentation of manuscripts-thesis writing- discussion of results.

References for I :

1. ‘Research Methodology’, Rajammal P.Devadas & K.Kulandaivel, 1979.

2. ‘Research Methodology’, C.R. Kothari New Delhi, Wiley Eastern Ltd, 1985.

3. ‘Research Methodology’, N.Gurumani, MJP Publishers First Edition.

II: NUMERICAL METHODS

1. Solution of differential equations –Euler’s method-Runge-Kutta method
2. Matrix algebra and simultaneous equations-elementary operations of matrices-gauss-Jordon elimination method-matrix inversion-Eigen values and Eigen vectors of real Symmetric matrix.
3. Differentiation and integration –Legendre polynomials-Gaussian quadrature-Interpolation-Lagrange interpolation.

References for II:

1. ‘Computer applications of Numerical Methods ‘,S.S.Kuo,Addison-Wesley,Massachusettes,1972.

2. ‘Computer oriented Numerical Methods ‘,V.Rajaraman,(2nd Edn.),PHI, New Delhi.

3. ‘Numerical Recipes in Fortran ‘, Press et al .,(2nd Edn.), Cambridge University Press ,1992.

4. ‘Numerical Methods ‘, E.Balagurusamy, TMH, 1999.

III: STATISTICAL METHODS

1. Least curve fitting-normal equations for curve fitting-orthogonal polynomials-Chebyshev polynomials.

2. Errors- Mean-standard deviation-moments-variance-skewness-distribution models-propagation of errors.

References for III :

1. ‘Statistics ‘, M.P.Spiegel,Schaum’s Outline series, (Asian Student Edn.),McGraw Hill,Singapore,1981.

2. ‘Computer oriented Numerical methods ‘,V.Rajaraman,(2nd Edn.),PHI, New Delhi,1980.

3. ‘Advanced Practical Physics ‘, M.Nelkon & J.M.Ogborn,(4th Edn.),ELBS,London,1977.

IV: COMPUTER PROGRAMMING

1.Introduction to computers-digital and analog types-binary arithmetic-inter- conversion between binary,decimal,octal and hexadecimal systems-binary coded decimal-8421 code-gray code-excess 3 code and inter- conversion.

2. FORTRAN-writing programs-data types-constants, variables and data structures-basic statements- input, output statements-sub-programs-additional features-applications.

3. BASIC-Introduction to structured programming-Basic statements-login, logout –error diagnostics- debugging-branching-library functions-vector matrix operations-applications.

Reference for IV:

1. 'Digital Computer Fundamentals', T.C.Bartee, (5^{th} Edn.Asian Student's Edn.), McGraw-Hill, Singapore, 1982.
2. 'Digital Logic and Computer Design ',M.M.Mano,Prentice-Hall India ,New Delhi, 1979
3. 'Programming in Basic ',E.Balagurusamy,TMH,New Delhi,1989
4. 'Basic Programming Self-Taught ', S.C.Hirsch, PHI, New Delhi, 1983.
5. 'Programming in Fortran 77', V.Rajaraman, TMH, New Delhi, 1981.
6. 'Programming with Fortran ', S.Lipschutz, Schaum's Outline Series 'McGraw-Hill, Singapore, 1988.

CORE PAPER II

Advanced Topic in physics – Credit - 6

I: QUANTUM MECHANICS

1.Vector space concepts-quantum states-dynamical variable as abstract vectors and operators-representations-transformation-diagonalisation and simultaneous diagonalisability-time evolution- Schrödinger, Heisenberg and interaction pictures-symmetries and conservation laws.

2. Relativistic wave equations-Klein-Gordon equation-plane wave solutions-Dirac equation-plane wave solutions-negative energy states-spin and magnetic moment of electron-particle-antiparticle formalism-elementary particles.

3. Angular momentum-quantum mechanical definitions-commutation rules-Eigen value spectrum-matrix representation-addition of two angular momenta-C-G coefficients-application to physical problems.

References for I:

1. 'A Text Book of Quantum Mechanics' .P.M.Mathews & K.Venkatesan, TMH, New Delhi, 1976.
2. 'Introduction to Quantum Theory'. D.Park, McGraw-Hill, Singapore, 1992.
3. 'Quantum Mechanics', E.Merzbacher, John Wiley & Sons, Singapore, 1970.

II: GROUP THEORY

1. Definition of groups, subgroups and classes-symmetry elements and symmetry operation-representation of symmetry operations by matrices-matrix representation of group-reducible and irreducible representation-character table-analysis of reducible representations-normal modes of various symmetry types.

References for II:

1. 'Elements of group Theory for Physicists', A.W.Joshi, (3rd Edn.), Wiley Eastern ltd., Chennai, 1982.
2. 'Chemical Applications of Group Theory', F.A.Cotton, (2nd Edn.), Wiley Eastern ltd., Chennai, 1971.
3. 'Group Theory and its Applications to Physical Problems', N.Hamermesh, Addison-Wesley, Massachusetts, 1964.

III: CHEMICAL PHYSICS

Molecular structure: Born –Oppenheimer approximation-hydrogen molecule ion-hydrogen molecule-valence bond method –molecular orbital method-structure of diatomic molecule-shape of polyatomic molecules.

1. Determination of molecular structure: X-ray diffraction-determination of molecular symmetry and molecular parameters-electron diffraction.
2. Molecular spectra: Types of transitions-rotation of diatomic molecules and polyatomic molecules-IR rotation-vibration spectra of gaseous diatomic and simple polyatomic molecules-theory of Raman intensities-bond polarisability derivatives-bond types from Raman intensities-bond orders.

References for III:

1. 'Molecular Quantum Mechanics', P.W.Atikins, (2nd Edn.), Oxford Univ.Press, London, 1982.
2. 'Fundamentals of Molecular Spectroscopy', C.N.Banwell & E.M.McCash, (4th Edn.), TMH, New Delhi, 1994.
3. 'Determination Molecular Structure', P.J.Wheatly.
4. 'Spectroscopy', B.P.S.traughan & S.Walker, Vols. 1&2, Chapman & hall, London, 1976.
5. 'Introduction to Molecular Spectroscopy', G.M.Barrow, McGraw-Hill, Tokyo, 1962.

ELECTIVE

X-ray Crystallography –Credit- 6

I: Crystal structure:

Crystal lattice- crystallographic axes-simple lattice (sc)- Body cubic (bcc)-face centered cubic (fcc)- Miller indices –crystal structure of sodium chloride-Hexagonal close packing –cubic close packing-coordination number –crystal packing factor –symmetry operation / elements ,Rotation-Transition –inversion symmetry-space groups-equivalent position in a unit cell- point groups – space groups.

II: Bonding in solids:

Covalent bond -ionic bonding- similarities and differences between ionic and covalent-Transition between covalent &ionic bonding –Metallic bond –bond order- bond length-bond energy-difference between polar bonds molecule-intermolecular attraction-vanderwals forces-

origin of vanderwals dispersion forces –temporary fluctuating dipoles –strength of dispersion forces-how molecular shape affects the strength of dispersion forces – dipole- dipole interaction in vanderwals forces- hydrogen bond- symmetric hydrogen bond- dihydrogenate bond- advanced theory of hydrogen bond –interaction to hydrogen bonding in water –hydrogen bonding in biomolecules.

III: Experimental Methods of X-ray Diffraction:

Reciprocal Lattice-Reciprocal lattice of various crystal systems-The Ewald Sphere-Electron in a Periodic Potential-Diffraction of X-rays by Crystal lattice-Laue's Formulation of X-ray Diffraction-X-ray Diffraction and Bragg's law-X-ray Diffraction methods-Laue Diffraction-Rotating crystal method-X-ray Powder Diffraction.

IV: Crystal Structure Determination:

Scattering factor –Structure factor-centro- symmetric crystal and the phase problem-need for phase-oscillation method of X-ray Diffraction-The Precession Method-X-ray Diffractometer-X-ray Source-Goniometer-Video camera (or) Microscope-X-ray Detector system-Host computer-Data collection-Determination of Structure factor-Steps in crystal structure determination-Electron Diffraction-Neutron Diffraction.

V: Crystal Structure Analysis:

Softwares for Crystallography-Structural analysis-Stereo Chemistry-Molecular structure and Chemical Bonding-Hybridization-Dihedral Angle-Chirality - Conformation of Acyclic and Cyclic systems.

References:

1. Elementary Crystallography – D. Velmurugan, MJP Publishers, 2008.

2. Elements of X-Ray Crystallography – Leonid. V. Azaroff, New York, McGraw Hill, 1968.

3. Stereochemistry of Organic Compounds – D. Nasipuri, John Wiley & sons, Chichester, 1991.

4. Stereochemistry – P.S. Kalsi, New age international, (6^{th} Edn) 2005.

5. Crystallography and its Application – Dent Glasser.L.S , Van Nostrand Reinhold ,1977.

6. Crystallography for Solid State Physics – Verma Ajit Ram & Srivastava, Wiley Eastern, 1982.

7. Essentials of Crystallography – M.A.Wahab. Narosa Book Distributors Private Limited, 2009.

8.Fundamentals of Crystallography – C. Giacovazzo, H.L. Monaco, G. Artioli, D. Viterbo, G. Ferraris, G. Gilli, G. Zanotti, M. Catti, Oxford University Press, USA, 2002.

ELECTIVE

CRYSTAL GROWTH- Credit-6

I: NUCLEATION

Nucleation concept – Kinds of nucleation – Classical theory of nucleation - Spherical nucleus – Induction period – Measurement - Heterogeneous nucleation – Equilibrium concentration of embryos – Energy of formation of a critical nucleus - Free energy of formation of a critical heterogeneous cap shaped and disc shaped nuclei –Nucleation rate - Secondary nucleation.

II: CRYSTAL GROWTH THEORIES

Surface energy theory – Diffusion theory – Adsorption layer theory – Volmer theory – Bravais theory – Kossel theory – Two dimensional nucleation theory – Free energy of formation

of a two dimensional nucleus – Possible shapes – Rate of nucleation – Mononuclear model – Polynuclear model – Birth and spread model – Modified Birth and spread model.

III: CRYSTAL GROWTH FROM SOLUTION

Low temperature solution growth – Solution and Solubility – Preparation of solution - Principle of low temperature solution growth - Mier's solubility diagram – Measurement of solubity – Measurement of Ostwald-Mier's metastable zone width – Achievement of supersaturation.

Crystal Growth methods – Slow cooling method – Holden's rotary crystallizer - Mason Jar method – Mastner and Janta method - Slow evaporation method – Johnson's rotating crystal method - Temperature gradient method – Kruger and Fink U tube method.

IV: MELT GROWTH AND VAPOUR GROWTH

Growth of crystal from melt – Bridgman method – Kyropolous method – Czochralski method – Verneuil method – Phase diagram principle of zone refining - Zone melting method – LEC growth of III – V materials.

Physical vapour deposition – Chemical vapour deposition – Open and closed systems – Physical and thermo-chemical factors affecting growth process.

V: GEL GROWTH, HYDROTHERMAL GROWTH AND FLUX GROWTH

Gel growth – Different gel medium – Specific gravity – Silica gel – Agar gel – Basic growth procedure – Single diffusion technique – Double diffusion technique – Reaction method – Chemical reduction method.

Crystal growth by hydrothermal method.

High temperature solution growth (Flux growth) – Principle of flux growth – Slow cooling method – Slow evaporation method – Top seeded solution growth.

BOOKS FOR STUDY

1. J. W. Mullin, "Crystallization

2. M. Ohora and R. C. Reid, “Modeling of Crystal Growth Rates from Solution”
3. J. C. Brice, “ Crystal Growth Processes”
4. J. C. Brice, “The Growth of Crystals from Melt”
5. D. Elwell and H. J. Scheel, “Crystal Growth from High Temperature Solution”
6. Heinz K. Henish, “Crystal Growth in Gels”, Cambridge University Press, 1973.
7. Crystal Growth techniques: P. Ramasamy & Santhana Raghavan

BOOK FOR REFERENCE

1. P. Ramasamy and F. D. Gnanam, “UGC Summer School Notes”. 1983.