

AWADHESH PRATAP SINGH UNIVERSITY, REWA (M.P.)



SYLLABUS FOR M.PHIL. CHEMISTRY TWO SEMESTERS (ONE YEAR COURSE)

M. Phil. (Chemistry) Ist Sem.
Paper-I
Computer for Chemists

Unit-I: Networking and search Internet

Historical background, Need & Advantage of computer network, Type of computer network, LAN, MAN, WAN, Basic HW & SW requirement for networking, Preliminary introduce of modem, can card, various communication media, HUB, Switches routers and gateway, Wireless network, The internet its application, WWW creation of web sites, searching and auessing information from web, using ftp & telnet.

Unit-II: Computers applications in Inorganic Chemistry

Shapes of ions and molecules using VSEPR theory Doppler shift and recoil velocity from Mössbauer data Concentration of complexes using Beer's Lamberts law Bonding energy of a nucleus d-orbital splitting in octahedral field Solubility of sparingly soluble salt

Unit-III: Computer application in Organic Chemistry

Synthesis of Organic compounds Dipole moments of disubstituted benzene Resonance energy for organic conjugated systems (Heat of combustion) Isoelectric point of amino acids ^{13}C chemical shift in organic compounds Woodward Hoffman rules in pericyclic reaction

Unit-IV: Computer application in Physical Chemistry

Determination of constants, a,b,g and axial ratio a':b':c' for crystals Delocalization energy for butadiene using Group theory. Symmetry numbers for molecules using data on symmetry operations Character table for C_{3v} point group Wave numbers of stokes and anti-stokes lines Parameters from NMR and ESR data

Books:

1. Computers in Chemistry, K V Raman; Tata McGraw-Hill Publishing.
2. Computers and Common Sence, R. Hunt and J. Shelley, Prentice Hall.
3. Computational Chemistry, A. C. Norris.
4. Internet Technology, V.K. Jain, DOEACC.
5. Computer Programming in FORTRAN IV, V. Rajaram, Prentice Hall.

M. Phil. (Chemistry) Ist Sem.

Paper-II

Unit-I (A) Polymer and Plastics

Introduction, Polymer synthesis, Polymers degradation, Photochemical degradation, Biodegradation of naturally occurring polymeric substances, Disposable synthetic polymers, Polymer recycling, Carry bags-A menace.

(B) Pesticides- Introduction, Chemistry of chlorinated organic compounds polychlorinated biphenyls (PCB), Insecticides, Pesticides interfering with respiration, Second generation pesticides, Lindane, Polychlorinated cyclopentadiene derivatives, Organophosphorus pesticides, Carbamates.

Unit-II Polymeric Inorganic Compounds I: Molecular Species

Introduction, Homoatomic inorganic polymers, Borazines, Silicones and related compounds, Phosphonitrilic polymers, Tetrasulphur tetranitride and related compounds, Coordination polymers. Polymeric Inorganic compounds

II: Polycations and Polyanions

Introduction, Polycations, Isopoly and heteropoly acids of transition metals, Silicates, 5 Borates, 6 Condensed phosphates.

Unit-III Enzymes

Introduction, Classification and nomenclature, Active sites and catalytic action, Allosteric activation, Regulation of enzyme activity, Covalent modification, Allosteric control, the specific nature of enzyme action, the mechanism of enzyme action, the general physical factors affecting enzyme action. Enzyme Kinetics: Single substrate reactions, Multiple substrate reactions, the sequential or single-displacement reactions, Double-displacement or ping-pong reaction.

Unit-IV Chemical Toxicology

Toxic chemicals in the environment, Impact of toxic chemicals on enzymes, Biochemical effect of Arsenic, Cadmium, Lead, Mercury, Carbon monoxide, Nitrogen oxides, Ozone and Pam, Cyanide, Pesticides, Carcinogens.

Books:

1. Modern Aspects of Inorganic Chemistry, Emelius and Sharpe, UBS.
2. Environmental Chemistry, P.S. Sindhu, New Age.
3. Medicinal Chemistry- An Introduction, Gareth Thomas, John Wiley and Sons, New York.
4. Environmental Chemistry, A.K. De, New Age.
5. Heavy Metals in the Environment- Bibudhendra Sarkar.

M. Phil. (Chemistry) Ist Sem.
Paper-III

Unit-I Combinatorial Chemistry

Introduction, The basic concept of Combinatorial Chemistry, The design of combinatorial syntheses, The general techniques used in Combinatorial.

Molecular structure: what is structure, Chemical graph, Aspects of atom level description electronic, satiric duealily of structure descriptors, Ramdic intrinsic state of an atom, delta values connectivity, Index, kier & Hall modification, E- state electronic in δ values intrinsic state algorithm, Higher quality level atoms, Field influence on the I state sample calculation CH_3-CH_2- , $\text{CH}_3-\text{CH}_2-\text{O}$, $\text{CH}_3-\text{CH}_2-\text{O}-\text{C}$, $\text{CH}_3-\text{CH}_2-\text{O}-\text{C}=\text{O}$, $\text{CH}_3-\text{CH}_2-\text{O}-\text{C}$,

Unit-II Drug Design

Introduction, Analogues and prodrugs, Concept of Lead (Examples), Factor governing Drug-Design, Relational approach to Drug-Design (Quantum mechanical approach, Molecular orbital approach, Molecular connectivity approach, Linear free energy approaches), Drug-Design: The Method of variation (Drug design through disjunction, Drug design through conjunction), Drug design and development: An overview (Problem, Revolution in drug discovery, Research and development strategies, Molecular hybridization, Rigidity and flexibility vs Drug design (Increased rigidity and increased flexibility), Tailoring of drugs.

Unit-III Physiochemical Aspects of Drugs

Introduction, Physical properties (Features governing drug action in active site, Structurally specific drugs, Structurally non-specific drigs, Thermodynamic activity, Mayer-Overtone and Mayer-Hemmi theory, Ferguson's theory, Van derwaal's constent, The Cut-off point, Steric factors, Hansch equation, The Craig plot, Verloop steric parameter), Factors governing ability of drugs to reach active site (Absorption, Distribution, Metabolism, Excretion, Intramolecular distances and biological activity), Dissociation constants (Drug exerting action on undissociated molecules, Drug exerting action on ionized molecules).

Unit-IV Biological Aspects of Drugs

Isosterism and Bio-Isosterism (Classical Bioisosteres, noncalssical Bioisosteres), Stereochemistry and drug action (Enantiomers, Diastereoisomers, Stereochemistry and Biological activity, Positional Isomers or Constitutional Isomers, Geometrical Isomers, Absolute Configuration, Easson-Stedman Theory, Conformationally flexible to Conformationally rigid molecule), Chemical Properties (Molecules negentropy, Cammarata correlation)

Books:

1. Medicinal chemistry; Ashutosh Kar, New age International Publisher.
2. Natural Products, Chemistry and Biological Significance, J. Mann, R.S. Davidson, J. B. Hobbs, D.V. Banthrope and J.B. Harborne, Longman, Essex.
3. New Trends in Natural Product Chemistry, Atta-ur-Rahman and M.I. Chaudhary Harwood Academic Publishers.
4. Organic Chemistry, Vol 2, I.L. Finar, ELBS
5. Molecular Structure descriptors, L.B. Kier & L.H. Hall , Acedamic Press.

M. Phil. in Chemistry Paper-IV IInd Sem.
Research Methodology

Unit-I Voltammetry and Polarography

Fundamental of Voltametry, Conventional or d.c. voltametry, Conventional or d.c. polarography, Theoretical principal, Complex ion, Quantitative techniques, The effect of oxygen, Simple polarography and classical d. c. polarography, The three electrode polarograph: potentiostatic control, Modified voltametry. Principal and instrumentation, Brief description of polarographic measurement, Current voltage relationship, Polarograms interpretation of polarographic waves. Equation for the polarographic waves, Half wave potential and its importance, The kinetic and catalytic currents, Polarographic cell, the dropping mercury electrode, Advantages of DME, Limitations of DME, The capillary and its care, Condition for performing polarographic determinations, Advantages of polarography, Application of polarography, Quantitative analysis, Qualitative analysis, Inorganic polarographic analysis, Organic polarographic analysis, Stationary electrode (slow linear scan) polarography, Cathode ray (rapid linear scan) polarography. Anodic stripping (inverse polarography), Alternating current polarography, Chronopotentiometry, Instrumentation and procedure, Application.

Unit-II Electrophoresis and Electro Chromatography

Definition, Types of electrophoretic methods, free solution electrophoresis, the Tiselius method, Moving boundary electrophoresis, Density gradient electrophoresis, Zone electrophoresis or electrochromatography, Types of supporting or stabilizing medium, Paper electrophoresis, Paper used, Electrode, Source of current, Location of component, Requirements of electrophoretic chambers, Problems in electrophoresis, Application of electrochromatography, Separation of serum proteins by paper electrophoresis, Separation of inorganic substance, Immunoelectrophoresis, Preparative electrophoresis on cellulose acetate, Electrophoresis in gels, Electrophoresis in powder.

Unit-III High Pressure (or Performance) Liquid Chromatography

Introduction, High performance liquid chromatography, Mode of chromatography, Principle and apparatus for HPLC, Solvent delivery system, Pumps, Sample injection

system, The column, Column packing materials, Column packing, Choice of supporting materials for a separation, TLC and HPLC, Detectors, Characteristics of detector, Some detectors used HPLC, Performance, Method, Identification of solute peaks, Quantitative HPLC, Accuracy and precision of HPLC, Materials, Advantages of HPLC, Effect of temperature in HPLC, Preparative HPLC, Important applications of HPLC, Inorganic chemistry, Forensic chemistry, Natural and synthetic pharmaceutical drugs, Steroids, Lipids, Alkaloids, Amino acids and proteins, Carbohydrates, Nucleic acids, Preservatives and antioxidants, Vitamins, Coal and oil products, Environmental pollutants, Pesticides.

Unit-IV Topological parameters

Topology

What are topological parameters?, Distance matrices of chain and classic graphs, Calculation of Wiener index , S_z index, Path number, PI index, Balaban index, in case of benzene, quinoline, acridine , pyridine and their derivatives

QSAR

Correlation analysis, Types of correlation, Calculation of variance, Rank Correlation, Regression analysis, linear regression line, Standard error of estimation, ANOVA, Pogliani's factor, Evaluation of some statistical parameters using activity data.

Books:

1. A Basic Course in Statistics: G.M. Clarke and D. Cooke; Second Ed. ELBS
2. Biostatistics: Arora and Malhan, Himalaya Publishing
3. Vogel's Textbook of Quantitative Chemical Analysis: J. Mendham, R.C.
4. Denney, J.D. Barnes, M.J.K. Thomas; Pearson Education
5. Instrumental Method of Analysis: Willard, Merit and Dean
6. Instrumental Method of Chemical Analysis: B.K. Sharma; Goel Pub. Meerut
7. QSAR and molecular modeling by S.P. Gupta, Springer Verlag, Germany
8. Hand book of molecular descriptor, Todeschini R. and Consonni V, Wiley, VCH, Weinheim.