

Paper I - Research Methodology

Unit I - Literature search:

Searching the chemical literature, primary sources - journals and patents, secondary sources (Beilstein, reviews, periodicals - serials - monograph and textbooks), dictionaries, encyclopedias, catalogues and index of tabulated data, location data, location of published and comprehensive account of research with special reference to physical, organic and inorganic chemistry (use of computer in literature search) significance of Chemdraw - drawing chemical structure - paste them in the text.

(Inductive and deductive reasoning - role of experimentation - interpretation of results - formation - testing and rejection of hypothesis - logic of scientific discovery)

Unit II - Error in chemical analysis and statistics:

(Classification of errors - accuracy - precision - minimization of errors - mean - standard deviation - Normal or Gaussian distribution - Reliability of results - confidence interval - comparison of results - Student's t-test, F test, paired t-test, correlation and regression) the least squares method for deriving calibration plots like straight line - (power curve - exponential curve - second degree parabola - (general methods used, standard addition, universal standard method - problems in these methods using least square fitting - quality assurance and control charts.)

Unit III - Computers in chemistry: (K. V. Ramani)

Data types: int, short, long int, float, double and long double; variable and scope. (Global automatic register) and static operators: assignment, caching, precedence and associativity: program selection: if-else logical operators - ternary operator switch statement: Repetition: while, do-while and for loops, goto statement; functions, void. Return statement, invoking functions, passing arguments - prototyping.

Array: Single dimensional arrays, accessing arrays, initializing and copying arrays - array as function arguments - multidimensional arrays.

(Simple C programming applications in chemistry such as van der Waals equation, pH titration, kinetics, radioactive decay, evaluation of lattice energy and ionic radii from experimental data)

Unit IV - Reaction mechanism:

(Methods of determining reaction mechanism: kinetic and non-kinetic methods - study of fast reactions - relaxation methods - flow techniques - Flash photolysis) - magnetic resonance methods for kinetic studies - reactions of radicals, electron transfer reactions, - mechanism of oxidation reactions involving metal ions and proxy anions - Michaelis-Menten kinetics - micellar catalysis - homogeneous catalysis: essential step in catalytic cycles involving transition metal complexes - properties of metals and ligands in homogeneous catalysis - selectivity in homogeneous catalysis.

(An introduction to linear free energy relationships. The Hammett equation - the quality of substituent and reaction constants and Yukawa-Tsuno equation. The general validity of the

Hammett equation - deviation from the Hammett equation in its various forms - non-linear Hammett plots - reactivity-selectivity principles.

Unit V - Instrumental method of analysis:

Basic instrumentation of IR, UV, NMR and EPR spectrophotometers - NMR spectroscopy - proton and ^{13}C - fluxional NMR - 2-dimensional NMR - uses of Shift reagents.

EPR spectroscopy - hyperfine splitting - factors affecting g value - anisotropy of g and A tensors - zero field splitting - Kramer's degeneracy - EPR spectra of Vanadium(III), Nickel(II) and Cu(II) complexes. Jahn-Teller distortion in Cu(II) complexes. Evaluation of bonding parameters.

Instrumentation, principles and application of (Cyclic Voltammetry) (93) }
NMR }
UV }

Combined applications of Mass, UV-Vis, IR and NMR leading to structural elucidation of simple organic compounds.

References:

Unit I

1. Advanced Organic Chemistry, Jerry March, 4th Edition.
2. How to find chemical information? A guide for practicing chemistry teachers and students, Robert E. Metz.

Unit II

1. Vogel's Textbook of Quantitative Chemical Analysis, V Edn., Longman Scientific and Industrial, UK, 1989.
2. Fundamentals of Analytical Chemistry, VII Edn., D.A.Skoog, D.M.West & P.J.Holler, Saunders College Publishing, New York (1996).

Unit III

1. Computers in Chemistry, K.V.Raman, Tata McGraw - Hill Publishing Co., Ltd., New Delhi (1993).
2. Programming in ANSI-C, II Edn., E.Balagurusamy, Tata McGraw - Hill Publishing Co., Ltd., New Delhi (1998).

Unit IV

1. Advanced Organic Chemistry, Jerry March, 4th Edition.
2. Reaction Mechanisms: A Guide Book, P.Sykes.
3. Structure and Mechanism in Organic Chemistry, E.S.Gould.
4. Chemical Kinetics, Frost and Pearson.
5. Electron Transfer Reaction, R.D.Canon. Butterworth.
6. Inventions of Rate and Mechanism of Reactions: Part 1, 2nd Edition, S.L.Fuess, E.S.Lewis and A.Weissberger.
7. Chemical Kinetics, K.J.Laidler.
8. Fast Reactions, Bradley.
9. Advances in Linear Free Energy Relationships, N.B.Chapman & J.Shorter.
10. Correlation Analysis in Organic Chemistry: An Introduction to LFER, J.Shorter.
11. Correlation Analysis in Organic Chemistry, N.B.Chapman & J.Shorter.

Unit V

1. H.V.Malmstadt, C.G. Enke and S.R.Crouch, Instrumentation for Scientists Series Modulas 1-4-Benhamin Inc.
2. Instrumentation Methods of analysis, Willard, Merrit & Dean.
3. Principles of Instrumental Analysis, D.A.Skoog & D.M.West.

4. NMR and Chemistry, J.W. Akitt, II Edn.,
5. Fourier Transform NMR Techniques: A Practical Approach, K. Mullie & P.S. Pregosin.
6. Data Reduction and Error Analysis for Physical Sciences, P.B. Berington, McGraw - Hill Book Company.
7. Applications of Organic Spectroscopy of Organic Compounds, J.R. Dyer.
8. Spectroscopic Identification of Organic Compounds, R.M. Silverstein, G.O. Bassder & T.C. Murrell.
9. Organic Spectroscopy, W. Kemp.
10. Physical Methods in Chemistry, R.S. Drago.

Paper II - Course Work

Unit I - Organic synthesis and organometallic reagents in synthesis:

Types of (carbon to carbon bond forming) reactions - key intermediates - starting materials - Sandheimer synthesis - Stork approach. Use of retrosynthetic analysis for the synthesis of simple cyclic molecules - Gabriel synthesis. A schematic analysis of the total synthesis of γ -caprolactone, 6-methoxy tryptamine, 6,6-ethylenedioxy-1(9)octalin-2-one, α -onocerin and quinotoxine. (Organo copper reagents - Vinyl Grignard reagents - carboalumination - nucleophilic addition of alkenylates and alkenylalanates to carbonyl compounds - ortho lithiation - use of formamidines - initiated dienes and nitroalkanes in synthesis.)

Unit II - Group theory:

Projection operators - symmetry adapted linear combination (SALC) - construction of MO wave functions for allyl, butadiene, cyclopropenyl, benzene and tetramethylcyclobutane - calculation of delocalization energies - (construction of hybrid orbitals and wave functions of hybrid orbitals for molecules having tetrahedral, trigonal triangular and square planar geometry (sp^2 , sp^3 and dsp^2 hybridizations). assignment NH_3, CH_4)

(Application of group theory to IR, Raman and UV spectroscopy - selection rules for fundamental vibrations - symmetry of normal vibrations of molecules belonging to C_{2h} , C_{2v} , C_{3v} , C_{4v} , D_{3h} , D_{4h} , $D_{\infty h}$ and $C_{\infty v}$ point groups, stretching mode analysis of metal carbonyls and metal complexes.)

Unit III - Bio-inorganic chemistry:

(Metalloproteins and enzymes. Blue copper proteins Copper proteins as oxidases/reductases - Nickel containing enzymes - structure of DNA - types of nucleic acid interactions - coordination, intercalation and hydrogen bonding - interactions of metal ions with nucleic acid - redox chemistry, hydrolytic chemistry - monitoring the DNA binding by UV, IR, NMR and CV spectral techniques. Applications of different metal complexes that bind nucleic acids - conformational probes - metallo foot printing reagents. Nature's use of metal/ nucleic acid interactions. Metal ion toxicity - detoxication using chelating agents. Inorganic compounds as therapeutic agents Anticancer drugs - antiarthritis drugs. Treatment of essential trace metal deficiencies and excess.)

Unit IV - Fundamentals of medicinal chemistry:

of block etc

Definitions of medicinal chemistry, pharmacology and molecular pharmacology. Major process involved in drug action - pharmacokinetics phase - quantitative structure activity relationship (QSAR) - Haunch approach. The concept of biostereism - pharmacodynamic phase - receptors and classification of membrane bound receptors - enzyme inhibitors as drugs (illustrated with one example). The concept of allosterism - (Agonist and antagonists - neurotransmitters in peripheral nervous system - cholinergic and adrenergic nerve transmission - relationship between drug metabolism and drug design - prodrugs and soft drugs.)

Unit V - Nanochemistry and photochemistry:

Nanoparticles and nanostructural materials - introduction - methods of preparation - physical properties - metallic behaviour - magnetic behaviour - optical and electronic properties - chemical properties of surfaces: metals - semiconductors - metal oxides - application of nanoparticles: water purification - catalysis - sensors - information storage - solar cells - environmental clean up.

Solar energy conversion - photoelectrochemical cells - water splitting - semiconductor solar cells.

References:

Unit I

1. Organic Synthesis, R.E.Ireland, Prentice Hall, 1969.
2. The Synthesis and Characterisation of Inorganic Compounds, W.L.Jolly.
3. Advanced Practical Inorganic Chemistry, D.M.Adams & J.B.Raynor.

Unit II

1. Chemical Application of Group Theory, F.A.Cotton.
2. Introductory Group Theory, Davison.
3. Physical Methods in Chemistry, R.S.Draco.
4. Group Theory in Chemistry, V.Ramakrishnan & M.S.Gopinathan.

Unit III

1. Bioinorganic Chemistry, Ivano Bertini, Harry B.Gray, Stephen J.Lippard and Joan Selverstone Valentine, Viva Books Pvt. Ltd., 1998.
2. Inorganic Chemistry: Principles of Structure and Reactivity, James E.Huheey.
3. J.Chem.Edn., November 1985.
4. Basic Inorganic Chemistry, F.A.Cotton & G.Wilkinson.
5. A textbook on Medicinal aspects of Bioinorganic Chemistry, A.K Das. CBS Publishers.
6. Environmental Chemistry, A.K.De, Wiley Eastern Ltd.,
7. Bioinorganic Chemistry, G.R.Chatwal and Ajay Kumar Bhagi, Himalaya Publishing House.

Unit IV

1. Medicinal Chemistry, G.L.Patrick, II edn., Oxford University Press, 2001.
2. Medicinal Chemistry - A Biochemical Approach, T.Nogradi, Oxford University Press, 2004.
3. Introductory Medicinal Chemistry, J.B.Taylor and P.D.Kennewell, Ellisworth Publishers, 1985.
4. Burger's Medicinal Chemistry, M.E.Wolf (Ed), 5th edn., John Wiley & Sons, 1995.
5. Medicinal Chemistry (Instant Notes), G.Patrick, Viva Books Pvt. Ltd., 2002 (Indian edition).
6. Principles of Medicinal Chemistry, W.O.Foye, Lee & Febiger, 1975.

Unit V

1. Nanoscale Materials in Chemistry, Kenneth J.Klabunde, John Wiley & Sons, Inc., Publication, 2001.

Optional Paper II - Advanced Inorganic Chemistry

Unit I - Inorganic Polymers: 33 x 6

General properties of inorganic polymers - classification - homoatomic - heteroatomic - condensation - addition polymers - coordination polymers. Glass transition temperature - phosphorus based polymers - polydimethoxy and polydiethoxy phosphazines - polyphosphoryl chlorides - polyphosphates - metaphosphates - polyphosphates cross linked phosphates - ultraphosphate glasses - borophosphate glasses - uses of phosphorus polymers - polymeric sulphur nitride - chalcogenide glasses - coordination polymers - chain polymers - two dimensional polymers - synthetic coordination polymers - polymers having phthalocyanine and related structure - polymers with bis chelating agents.

Unit II - Molecular rearrangements and reactions of coordinated ligands:

Molecular rearrangements of four coordinated complexes - six coordinated complexes - reactions at coordinated ligands - reactions due to metal ion polarization of coordinated ligands - reactions due to metal-ion polarization of coordinated ligands - hydrolysis of amino acid esters and amides and of peptides - Aldol condensation - imine formation, hydrolysis and substituent exchange - the template effect and macrocyclic ligands.

Unit III - Organometallic compounds: 4.5.2

Alkylidene and alkylidyne complexes - synthesis of alkylidene complexes in low oxidation state and higher oxidation state of metals - synthesis of alkylidyne complexes - reactivity and bonding in alkylidene and alkylidyne complexes - alkyne complexes - synthesis, reactivity and bonding - cobalt catalysed alkyne cycloaddition reactions.

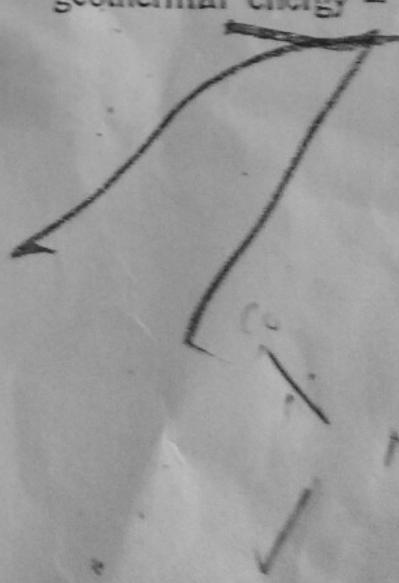
Unit IV - Metal ions in medicine:

Introduction - trace elements - metal deficiency and disease - toxic effect of metals (Pb, Cd, Hg and As) and their detoxification - metals used for diagnosis and chemotherapy - platinum anticancer drugs: discovery, principles and development of drug - clinical picture of cisplatin and carboplatin - Bioinorganic chemistry of platinum anticancer drugs - design of new inorganic anticancer drugs.

Unit V - Energy and environment: 9

Sources of energy - fossil fuels - nuclear fission - nuclear fusion - solar energy - use of solar energy in space heating and water heating - production of electricity using solar energy - solar trough collectors - power tower - solar bond - solar energy for driving vehicles - power from indirect solar energy - hydropower, wind power, biomass energy - product of ethanol, methane from biomass - photosynthesis - photoelectrochemical cells - geothermal energy - ocean thermal energy conversion - tidal power, air energy.

Energy conversion & storage.
electric cell.
photo electro spectroscopy



References:

Unit I

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1. Principles of Inorganic Chemistry, B.R.Puri, L.R.Sharma and K.C.Kalia, Milestone Publishers, Delhi, 30th edition.
2. Advanced Inorganic Chemistry, Gurdeepraj, Goel Publishing House.

Unit II

1. Inorganic Chemistry, K.F.Purcell and J.C.Kotz.

Unit III

1. Organometallic Chemistry, R.C.Mehrotra and A.Singh.
2. Organometallics I – Complexes with transition metal carbon s-bonds – Manfred Bochmann.

Unit IV

1. Bioinorganic Chemistry, Ivano Bertini, Harry B.Gray, Stephen J.Lippard and Joan Selverstone Valentine, Viva Books Pvt. Ltd., 1998.
2. Environmental Chemistry, A.K.De, Wiley Eastern Ltd.,
3. A textbook on Medicinal aspects of Bioinorganic Chemistry, A.K Das, CBS Publishers.

Unit V

1. A textbook of environmental chemistry and pollution control, S.S.Dara, S.Chand & Co., 7th edition.