

Ph.D. (Chemistry)

Techniques in Chemistry

Max. Marks: 80

Time: 3 hrs.

Note: Examiner will set 09 questions and the candidates will be required to attempt 05 questions in all. Question number 01 will be compulsory containing 08 short answer type questions covering the entire syllabus. Further, examiner will set 02 questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks

Section A

Purification/ Crystallization

Isolation and purification of organic compounds (solids and liquids) with special emphasis on chromatographic techniques: TLC, column chromatography and HPLC. Drying and dehydrating agents.

Section B

Spectroscopic Techniques

Theory and applications of NMR spectroscopy of H-1, C-13, N-15, P-31 nuclei, two-dimensional NMR spectroscopy, theory and applications of infrared and mass spectrometry of organic compounds.

Section C

Thermal Techniques

Differential Thermal Analysis (DTA): Theories of DTA, factors affecting DTA curves, instrumentation and application of DTA.

Thermogravimetry (TG): Instrumentation and balances, X'- Y' recorder, thermogram, factors affecting thermogram, correlation of DTA and TGA data.

Section-D

Measurement of Thermodynamic Properties

Excess molar volume; dilatometric and density measurement methods.

Excess molar enthalpies, Adiabatic, Isothermal, flow calorimeters.

Gibbs free energy of mixtures ; Marsh as well as Gibb's and VAN Ness static vapour methods for measuring vapour pressure of liquid and hence Gibb's free energy of mixing.

Excess isentropic compressibility ; Tecqniques for measuring speed of sound by DSA and Interferrometer ;determination of excess isentropic compressibilities.

Books suggested:

1. A textbook of Quantitative Inorganic Analysis, A.I. Vogel, ELBS, London.
2. Dynamics of Chromatography- Part I; J.C. Gidding; Dekker, New York.
3. Vogel's textbook of practical Organic Chemistry, B.S. Furhen ey. al. Longman Group.
4. Spectrometric Identification of Organic Compounds, R.M. Silverstein, G.C. Bassler and T.C. Morrill.
5. Spectrometric Methods in Organic Chemistry, D.H. Williams and I. Fleming.
6. Organic Spectroscopy, William Kemp, John Wiley.

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Inorganic Chemistry (Optional)

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Section A

Electro analytical Techniques

Polargraphy:- Introduction and Basic Principles, Polarograph, Polarographic cells, Half wave Potential and its significance.

DME:- Advantages and Disadvantages of DME, SCE

Carbon electrodes-Carbon paste Electrode

Types of Currents:- Diffusion Current, Migration Current, Kinetic Currents, Catalytic Currents, Limiting Currents

Amperometry :- Principles and Applications

Square Wave Polarography, Voltametry, Coulometry, Superimposed

AC Polarography:- Principles, theory and applications of these techniques.

Section-B

Nanomaterials:- Definition, Methods of Preparation

Properties of Nanomaterials:- Physio-chemical and optical, Electrical and Electronics properties.

Applications of Nanomaterials

Gold, Silver & Pt Nanomaterials:- General Properties and Applications

Section-C

Phosphorescent Materials

Luminescence, Types of Luminescence, Fluorescence, Phosphorescence, Frank

Condon Principle, Jablouski diagram, Organic Electroluminescence, Organic

Light Emitting diode, Structure and working of OLED, Applications of OLED

Inorganic phosphorescent materials, Long Persistent phosphors phosphors for

LED, Applications of Inorganic Phosphors

Section -D

Organometallic Compounds of Main Group Elements:

General characteristics of different types of main group organometallics, stability, routes of M-C bond formation: Oxidative addition, transmetallation,

6

Carbanion halide exchange, metal-hydrogen exchange, metal hydride addition to alkenes, methylenations and by Aryl diazonium salts.

Structure elucidation by spectral techniques like IR, NMR, Mossbauer for compound of Si, Ge, Sn, Pb, As, Sb, Bi and Te.

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Physical Chemistry (optional)

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Section-A

Thermodynamics of liquid mixtures

Molecular interactions in liquid mixtures: Ion-ion interactions, Ion-dipole interactions, Dipole-dipole interactions, Ion-induced dipole interactions, Dipole-induced dipole interactions, Quadruple-octuple interactions; specific interactions, hydrogen bonding, charge-transfer interactions and contact charge-transfer interaction. Thermodynamic of excess functions; excess molar volumes, excess molar enthalpies, excess isentropic compressibilities, excess Gibbs free energy, excess heat capacity and their significance. Statistical theories of liquid mixtures; (i) Cell model (ii) Flory's theory (iii) Sanchez and Lacombe's theory.

Section-B

Quantum mechanics

The Born-Oppenheimer approximation, The Hellmann-Feynman theorem, Huckel molecular orbital (HMO) theory. Applications of HMO theory (i) to set up and solve secular equation ; (ii) to calculate resonance energy; (iii) to draw molecular orbital energy diagram for (1) Ethylene molecule taking in to consideration the overlap integral and (2) Pyrrole molecule. Determination of resonance integral, " β " in HMO theory by (1) Ionization potential; (2) Electronic spectra and (3) delocalization energy methods.

Section-C

Solid State Chemistry:

Defects in crystals; Various types of defects in crystal; Thermodynamics of Schottky and Frenkel defects formation; Colour centers; Non-stoichiometric defects; Classification of solids; lattice energy; evaluation of Madelung constant (NaCl); calculation of repulsive potential exponent; Lattice heat capacity; Einstein and Debye model of lattice heat capacity; Debye T³ law.

Section D

Electrode:

Electron transfer under an interfacial electrical field; Butler-Volmer equation; electrode kinetic involving semiconductor solution interface; photoelectrochemistry; p-type photo-cathodes; n-type photo-anodes; Rate determining step in photo-electrochemical reaction; Ionic conductivity in solids; Solid electrolytes; Fast-ion conductors, oxygen ion conductors, sodium ion conductors;

Solid state ionic devices, Batteries: Lithium batteries; Sodium batteries; fuel cells; sensors.

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Organic Chemistry (Optional)

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Section – A

Stereo selective Synthesis

Principle of stereo selectivity, 1,2- and 1,3-asymmetric induction, acyclic stereoselection, distereoselection in cyclic systems.

Enantioselective synthesis: Enantioselective hydroboration, hydrogeantion, epoxidation, enantioselective synthesis via hydrazones.

Role of enzymes in chiral synthesis.

Section - B

Disconnection approach of synthesis

Introduction, main synthetic strategies, Synthetic strategies of 1,2- and 1,4-difunctionalised compounds, Group disconnection, Umpolung Strategies, α -functionalisation of carbonyl compounds. Synthetic approach to cyclic systems. Retro synthetic and reconnection strategies.

Reagents

Preparation and application of following reagents:

Hypervalent iodine, organoboron reagents (IBBN, CATB, IpC2BH, PINB), Organosilicon compounds, Trifluoromethyl sulphonates (triflates).

Section – C

Heterocyclic compounds

General synthesis of

(a) compounds with three or more heteroatoms in the ring

(1,2,3)- and (1,2,4)-triazoles

(1,2,4)- and (1,3,4)-oxadiazoles

(1,2,5)- and (1,3,4)-thiadiazoles

(1,2,3)-, (1,2,4)- and (1,3,5)-triazines.

Tetrazoles and tetrazines.

(b) Bridgehead nitrogen containing compounds:

Indolines

Imidazo [1,2-a] and [1,5-a]pyridines

Triazolo [1,5-a] pyridines

S-triazolo [3,4-b] [1,3,4] thiadiazoles

Imidazo [2,1-b] [1,3,4] thiadiazoles

S-triazolo [3,4-b] [1,3,4] thiadiazines

Thiazolo [3,2-b] [1,2,4] triazoles.

Section – D

Green Chemistry

Basic principles of green chemistry, Application of non-conventional techniques in organic synthesis (ultrasonic, microwave and grinding). Solid state synthesis and synthesis under solvent free conditions. Use of ionic liquids.

Drug discovery and development

A rational approach to drug design and drug development of following drugs:

cimetidine

oxamniquine.

Books recommended:

1. Asymmetric Synthesis Ed. J, D. Morrison, vol. 1-5. Academic Press.
2. Stereochemistry of Organic Compounds by D. Nasipuri.
3. Designing organic synthesis by S. Waren.
4. Heterocyclic Chemistry by T. L. Gilchrist.
5. Comprehensive Heterocyclic Chemistry by A. R. Katritzky and C. W. Rees.
6. Green Chemistry by M. Kidwai and V. K. Ahluwalia.
7. Wilson and Gisvold's Text Book of organic medicinal and pharmaceutical chemistry Ed. R. F. Dorge.