

## **DEPARTMENT OF CHEMISTRY**

### **Ph.D. Chemistry Course Work**

**(One Semester Course)**

**Scheme of Examination**

**w.e.f. January, 2017**

<b>Paper No/Code.</b>	<b>Nomenclature</b>	<b>Load</b>	<b>Credit</b>	<b>Maximum Marks</b>
Paper –I 17CHEPC1	Research Methodology	4 hrs/week	4	100 (80+20)*
Paper-II 17CHEPC2	Techniques in Chemistry	4 hrs/week	4	100 (80+20)*
Paper-III 17CHEPC31 17CHEPC32 17CHEPC33 (one optional out of three)	(i) Inorganic Chemistry (Optional) (ii) Physical Chemistry (Optional) (iii) Organic Chemistry (Optional)	4 hrs/week	4	100 (80+20)*

Each candidate has to study two compulsory (Paper I and II) and one optional (Paper-III one of the three optional i.e. Inorganic Chemistry, Physical Chemistry or Organic Chemistry). Each paper will be of 100 marks (04 credits) and will have a teaching load of 4 hrs/week.

\* Marks for Internal Assessment = 20. The internal assessment in each paper shall be based on assignment(s) and seminar(s) presented by each candidate and their participation

**PhD (Chemistry)**  
**Paper-I**  
**Research Methodology**

*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**

**Research Methodology:** Meaning, Scope, Primary sources of literature survey, Journals, patents etc., secondary sources of literature survey, Books, Reference books, Text books, listing of letters.

**Chemical Literature:** (1) The structure of chemical information, Important paper based and electronic based sources, How to find chemical information on specific compounds and their synthesis; (2) Abstracts and Journals in chemistry, Electronic forms of Journals, major libraries, subscribing Journals related to chemistry in the region and country; and (3) Patents and Patents writing, Parts of patent applications characteristics of the disclosure for a chemistry invention.

**Section B**

**Scientific Writing:** Scientific Document; Organization and writing of research paper, short communications, review articles, monographs, technical and survey reports, authored books, and edited books and dissertation.

**Section C**

**Internet and Web programming:** Hardware and software requirement for internet, ISP and internet account, Web home page, URL, Browser, Security on web, searching tools and search engines, FTP, Gopher, Telnet, e-mail and application of internet. Creating a web page, Text formation and alignment, Font control, Arranging text in lists, Images on web pages, Background and color control, Interactive layouts and frames.

**Section D**

**C++ Programming:** Constants, variables, data types, declaration of variables, user defined declaration, operators, hierarchy of arithmetic operators, expression and statements. Control statements: If, switch, conditional operator, go to, if- else. Decision making and looping statement: While, do-while, for, built in functions and program structure input and out put statement. Pointers and arrays.

**Ph.D. (Chemistry)**  
**Paper – II**  
**Techniques in Chemistry**

*Max. Marks: 80*  
*Time: 3 hrs.*

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**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 Interferometer ;determination of excess isentropic compressibilitys.

**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.

**Ph.D. (Chemistry)**  
**Paper-III (i)**  
**Inorganic Chemistry (Optional)**

*Max. Marks: 80*

*Time: 3 hrs.*

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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 Persistant 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, 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.

**PhD (Chemistry)**  
**Paper-III (ii)**  
**Physical Chemistry (optional)**

*Max. Marks: 80 Time: 3 hrs.*

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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, " $\beta$ " 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  $T^3$  law.

## **Section D**

### **Electrode:**

Electron transfer under an interfacial electrical field; Butler-Volmer equation; electrode kinetic involving semiconductor solution interface; photo-electrochemistry; 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.

**Ph.D. (Chemistry)**  
**Paper – III (iii)**  
**Organic Chemistry (Optional)**

*Max. Marks: 80    Time: 3 hrs.*

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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,  $\alpha$ -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,  $\text{IpC}_2\text{BH}$ , 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. Dorje.

