DEPARTMENT OF CHEMISTRY

Ph.D. Chemistry Course Work

(One Semester Course)

Scheme of Examination

W.e.f January,2017 to Deacember,2017

Paper No.	Nomenclature	Load	Maximum Marks
Paper –I 17CHEPC1	Research Methodology	4 hrs/week	100 (80+20)*
Paper-II 17CHEPC2	Techniques in Chemistry	4 hrs/week	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	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 credit) 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.

Program specific outcomes

PSO1 Analyse the literature survey, research paper writing, data interpretation, through computer programming.
PSO2 Understand the identification & purification of compounds by various techniques.
PSO3 Analyse the measurement of various thermodynamic properties.
PSO4 To know about the Nanoparticles, Phosphorescent Materials, Electroanalytical techniques and Organometallic compounds.
PSO5 Understand the Quantum mechanics, Thermodynamic excess functions, Crystal defects and Photo-electro chemistry.
PSO6 To know about Reagents in organic synthesis, Heterocyclic compounds, Drugs and techniques of Green chemistry.

PhD (Chemistry)

Paper- I (17CHEPC1)

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*

Course outcomes

CO1 To know the literature survey through books, journals , patents, References etc.
CO2 Understand the C++ Programming.
CO3 To learn the research paper writing .
CO4 Understand the Internet and Web programming.

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, Back ground 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 (17CHEPC1)
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***

Course outcomes

CO1 Deliver the importance of general spectroscopic techniques.
CO2 Explain the principles of the most important liquid chromatography.
CO3 Acquire some technical knowledge of TLC, column chromatography and HPLC.
CO4 Interpretation of Thermal Spectra (Thermogram) of the given sample by DTA/TGA
CO5 Understand the thermodynamic of excess functions and their significance

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 ; Tecqniqes for measuring speed of sound by DSA and Interferrometer ;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) 17CHEPC31

Inorganic Chemistry (Optional)

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***

Course outcomes

CO1 Know the processing of some nanoprticles,their properties and applications.
CO2 Understand the polarographic cell and various electrodes related to it.
CO3 Describe the process of performing an amperometric titration.
CO4 Be able to understand the applications of inorganic and organic Phosphorescent Materials.
CO5 To identify various organometallics and explained their synthesis and stability.

Section A

Electro analytical Techniques

Polagraphy**:-** 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

<u>Phosphorescent Materials</u>

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) 17CHEPC32
Physical Chemistry (optional)

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***

Course outcomes

CO1 Various concepts of quantum mechanics and their applicaitons.
CO2 Apply Huckels method for the determination of energies of conjugated hydrocarbon systems like ethylene, pyrrole etc.
CO3 Understand the thermodynamic of excess functions and their significance.
CO4 To know about the various types of defects in crystals.
CO5 Describe the photo-electrochemistry and different batteries.

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 T^3 low.

Section D

Electrodics:

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) 17CHEPC33
Organic Chemistry (Optional)

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***

Course outcomes

CO1 Apply different reagents in the organic transformations.
CO2 Understand the nomenclature, synthesis and reactivity of different heterocyclic compounds.
CO3 To know the drug design and development of cimetidine and oxamniquine drug.
CO4 To know the principles and techniques of green chemistry.

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-difuntionalised 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, IpC_2BH, 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 Cchemistry 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.