# Department of Chemistry Ch. Devi Lal University Sirsa

Ph. D. in the subject of Chemistry

Syllabi and Course of reading for Ph. D. (Course Work) in Chemistry w.e.f. 2018-49.

Paper No.	Course Code	Nomenclature of the Paper	Contact Hours (L+P)	Credits	Max. Marks
Paper-I	CH(H)-501	Research Methodology	4+0=4	4	70+30
Paper-II	CH(H)-502	Instrumental Methods in Chemistry	4+0=4	4	70+30
Paper-III	CHI(S)-503	Inorganic Chemistry	4+()=4	4	70+30
	CHO(S)-503	Organic Chemistry	4+()=4	4	70+30
	CHP(S)-503	Physical Chemistry	4+()=4	4	70+30
Total Max. marks					300

#### Note:

- CH (H), CH (S) represents Hard core, Soft core papers in Chemistry.
- Each theory paper will include 30% marks as internal assessment as per University rules.
- Maximum marks of will be 300.
- Total credits: 12 (Hard Core = 08; Soft Course = 04)
- Paper III is optional and candidates are required to select any one of the three specialization paper offered.
- A student is required to score 50 percent marks in aggregate in order to pass the theory examination. Pass marks in individual course is 45 percent.

# Instruction for the paper setters:

The examiner will set nine questions and the candidates will be required to attempt five questions in all. Out of nine questions one question will be compulsory containing seven short answer type questions covering the entire syllabus. Further examiner will set two questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks.

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## Paper-I Research Methodology CH(H)-501

Max. Marks: 70

#### Section-A

#### Scientific Writing

Scientific Documents: Organization and writing of research paper, short communications, review articles, monographs, technical and survey reports, authored hooks, and edited books and dissertation.

#### Chemical Literature

- a. The structure of chemical information, Important paper based and electronic based sources. How to find chemical information on specific compounds and their syntheses.
- b. Abstracts and Journals in chemistry, floppy forms of Journals, major libraries, subscribing Journals related to chemistry in the region and country.
- c. Patents and Patents writing :Parts of patent applications, characteristics of the disclosure for a chemistry invention.

#### Section-B

### Classification of analytical methods

Classical & Instrumental, Types of instrumental analysis selecting an analytical method, analytical balance, technique of weighing, errors, Selecting and handling of reagent. Safety in analytical laboratory.

Errors and Evaluation: Definition of term in mean and median, Precision, standard deviation, relative standard deviation, accuracy, absolute error, relative error. Types of error in experimental data. Determinate (Systematic), indeterminate (or random) and gross source of errors and effects upon the analytical results. Methods for reporting analytical data-indeterminate errors. Use of statistics.

#### Section-C

### The Purification of common organic solvents

Saturated aliphatic hydrocarbons, aromatic hydrocarbons, halogenated hydrocarbons, aliphatic alcohols, ethers, ketones, esters, nitropen containing solvents, sulphurcontaining olvents, phosphorus containing solvents.

#### Section D

### Identification of compounds on basis of different spectroscopic techniques

NMR spectroscopy ( $^{1}H$  and  $^{13}C$ ) techniques,mass spectrometery. UV-Vis spectroscopy, infraredspectroscopy.

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### Suggested readings

- 1. A Text book of Quantitative Analysis, A. I. Vogel, ELBS, London.
- 2. Fundamentals of Analytical Chemistry, D. A. Skoog, D. M. West & F J Holler, W. B. Saunders.
- 3. Analytical Chemistry: Principles and Techniques, L. G. Hargis, Prentice Hall.
- 4. Vogel's Text book of Practical Organic Chemistry, B. S. Furniss et. al., Longman group.
- 5. Spectroscopic Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Morrill.
- 6. Spectroscopic Methods in Organic Chemistry, D. H. Williams and I. Fleming, Tata McGraw Hill.
- 7. Organic Spectroscopy, William Kemp, John Willey.
- 8. How to write and publish a scientific paper, R. A. Day, Philadelphia, IST Press,
- 9. Scientific and Technical papers, S. F. Tribease, MIT Press, Cambridge, Mass and London England.

10. Effective writing for Engineers, Managers, Scientists, Tichy, A. L. Wiley, New York and London.

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## Paper-II Instrumental Methods in Chemistry CH(H)-502

Max. Marks: 70

#### Section-A

## Chromatographic Techniques

### i) Ion Exchange

Ion exchangers (synthetic and natural), ion-exchange equilibria, experimental technique, applications.

## ii) Gas Chromatography

Principle, theory of gas chromatography, GSC, GLC, HPLC, instrumentation, detectors used in gas chromatography, evaluation of gas chromatogram, identification of gas chromatogram, application of gas chromatography.

## iii) HPCL (High-Performance Liquid Chromatography)

Instrumentation, liquid chromatography (LC)/mass spectrometry (MS) and LC/MS/NS, high-performance partition chromatography, high-performance adsorption chromatography, ion-exchange chromatography, size-exclusion chromatography.

Buckyballs: The chromatographic eparation of fullcrenes, affinity chromatography, chiral chromatography, comparison of high performance liquid and gas chromatography.

#### Section-B

#### Thermal Techniques

Differential thermal analysis (DTA): Theories of DTA, factors affecting DTA curves, instrumentation and applications of DTA. Thermogravimetry (TG): Instrumentation and balances X'- Y' recorder, thermogram, factors effecting thermogram, Correlation of DTA and TGA data. Differential scanning calorimetry (DSC): Introduction and instrumentation, DSC curve, factors effecting DSC curve.

#### Section-C

### MoeeularFluorescene Spectroscopy

Theory of molecular fluorescence, effect of concentration on fluorescence intensity, fluorescence instruments, applications of fluorescence methods, use of fluorescence probes in neurobiology, probing the enlightened mind, molecular phosphorescence spectroscopy, chemiluminescencemethods.

## Section-D

## Applications of the following Analytical Techniques

Atomic absorptionspectroscopy, conductometry, spectrophotometery, flame photometry, cliabatometry.

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## Suggested readings

- 1. A Text book of Quantitative Inorganic Analysis, A. I. Vogel, ELBS, London.
- 2. Dynamics of Chromatography Part-I, J. C. Gidding, Dekker, New York.
- 3. Instrumental Methods of Analysis, L. L. Merrit, R. H. Willard and J. Dean, Van Nostrand-Reinhold.
- 4. Instrumental Methods of Chemical Analysis, H. Haur, Pragati Prakashan.
- 5. Vogel's Text book of Practical Organic Chemistry, B. S. Furniss et al, Longman group.
- 6. Spectroscopic Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Morrill.
- 7. Spectroscopic Methods in Organic Chemistry, D. H. Williams and I. Fleming, Tata McGraw Hill.
- 8. Organic Spectroscopy, William Kemp, John Willey.

9. Advanced Practical Organic Chemistry, J. Leonard, B. Lygo and G. Proetor, Stanely Thornes.

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## Paper-III Inorganic Chemistry CHI(S)-503

Max. Marks: 70

#### Section-A

#### Metal and Hetero bimetallic Alkoxides

Formation of metal-alkoxide bond.formation of hetero metallic alkoxide thewis acid-base reactions, condensation reactions, misc dianeous reactions. Characterization of metal and hetero bimetallic alkoxides using analytical and spectral methods. Structures of metal and hetero bimetallic alkoxides. Reactivity of alkoxide bond-alcoholysis, reactions with β-diketones, hydrolysis, transmetalation reactions, activation of small molecules like oxygen, catalytic activity. Molecular precursors of inorganic material for sol-gel and MOCVD applications

#### Section-B

## Organometallic compounds of main group elements

Introduction, classification, nomenclature and characteristic of organometallic compounds. Stability, metal exchange, metalhesis, metal halogen exchange, metalation, mercuration, hydrometallation, carbometallation, surbine insertion and decarboxylation reactions and structures of low-valent. Sigma bonoci organometallics multiple bonded silicon and arsenic organometallics,  $\beta$  cyclopentadienly i complexes of main group elements, structure elucidation through spectroscopic techniques and application of main group organimetallic compounds.

#### Section\_C

#### Reactions of organometallic transition metals

Oxidative addition and reductive elemention three centre additions, Sn<sup>2</sup> reactions, radical mechanisms, ionic mechanisms, reductive elimination, oxidative coupling and securitive extrusion, Insertion and elimination reactions; reactions involving CO, insertions involving alkenes, other insertions,  $\alpha$ - $\beta$ - $\gamma$ -and  $\alpha$ -climination. Nucleophilic and electrophilic additions and abstraction nucleophilic addition to CO nucleophilic additions to polyene and polyeny broands, nucleophilic abstraction in alkyls, cleanophilic addition to metal, electrophilic abstraction of alkyl groups, single electron transfer polyways.

#### Section-D

#### Analytical Chemistry

Use of organic reapents in moteranic analysis; oxine and its derivatives, sodium diethyldithiocarbamate, authiazone.cog (που.οχίσμες, β dil ctones.

Ion-exchange chromatography; ion exchange packings, experimental techniques, applications of Jon-exchange method.Radiochemical methods: Radioactive isotopes, instrumentation neutron activation, methods, isotopic dilution in thods.

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### Suggested readings

- 1. The Chemistry of Metal Alkoxides, N. Y. Turova, E. P. Turevskaya, V. G. Kessler, M. I. Yanovskaya, Springer US.
- 2. Metal Alkoxides, D. C. Bradley, R. C. Mehrotra and D. P. Gaur, Academic Press. London.
- 3. Principle and Application of Organotransition Metal Chemistry, J. P. Collman, L. S. Hegdus, J. R. Norton and R. O. Finke, University Science Books.
- 4. The Organometallic Chemistry of Transition Metals, R. H. Crabtree, John Wiley, New York.
- 5. Instrumental Methods of Analysis, L. L. Merrit, R. H. Willard and J. Dean, Van Nostrand-Reinhold.
- 6. Instrumental Methods of Chemical Analysis, H. Haur, Pragati Prakashan.

7. Fundamentals of Analytical Chemistry, D. A. Skoog, D. M. West & F.J.Holler, W. B. Saunders. 11/10 / 1/16 - 1/1/16.

## Paper-III Organic Chemistry CHO(S)-503

# Max. Marks : 70

## Stereochemistry

Stereoisomer: Separation, resolution and racemization, stereoselective synthesis, categories, Convergent synthesis, Diastereoselective synthesis of achiral compounds cyclones and alkenes, strategies of stereocontrol. Enantioselective synthesis with chiral reagents and catalysts. Chirotopical properties, Anisotropy

### Section-B

Section-A

## Reagents

Preparation, properties and application of the following reagents in organic synthesis: Phosphorus and sulfur ylides, hypervalent iodine and silicon compounds, Boronating agents- 9-BBN and Ipc<sub>2</sub>BH, Organocuperates.

#### Section-C

## Heterocyclic Compounds

Methods of synthesis and reactions including mechanism of the following: Three membered heterocycles: Aziridines, Oxiranes, Thiiranes, Four membered heterocycles: Azetidines, Oxetanes, Thietanes, Seven membered heterocycles: Azepines, Thiepines, Oxepines, Diazepines, Thiazepines,

### Section-D

## Supramolecular Chemistry

Properties of covalent bonds, bond parameters, polarizability, bond dissociation enthalpy and entropy, Intermolecular forces and hydrophobic effects. Electrostatic induction dispersion and resonance energy, Magnitude of interaction energy, forces between macroscopic bodies, medium effects, hydrogen bond.

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## Suggested readings

- 1. Asymmetric Synthesis, Ed. J. D. Morrison, Academic Press, New York, Vol. 1-5 (1985).
- 2. Principles of Organic Synthesis R. O. C. Norman and J. M. Coxon. Blackie Andemic and Professional.
- 3. Heterocyclic Chemistry, T. L. Gilchrist, Longman Scientific and Technical.
- 4. Heterocyclic Chemistry, Ed. Wiessberger, John Wiley Interscience Publication.
- 5. Comprehensive Heterocyclic Chemistry: The Structure, reactions, synthesis and uses of heterocyclic compounds, Vol. 7. Eds. A. R. Katritzky and C. W. Rees, Pergamon Press.
- 6. Some Modern Methods of Organic Synthesis, W. Carruthers, Cambridge University Press.

7. Supramolecular Chemistry, Concepts and Perspectives, J. M. Lehn, VCII.

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## Paper-III (Physical Chemistry) CHP(S)-503

Max. Marks: 70

#### Section-A

#### Partition function

Translational, rotational, vibrational and electronic partition and functions, calculation of thermodynamic properties in terms of partition functions, chemical equilibria and equilibrium constant in terms of partition functions. Application of statistical mechanics to chemical reaction kinetics.

#### Section-B

### Solid State Chemistry

Thermal decomposition, nucleation, free energy of nucleation, laws, classification, functions and growth of nuclei, kinetic expression for diffusion controlled reactions, phase boundary controlled and nucleation and growth controlled reactions. Defects in crystals, various types of defects, thermodynamics of schotky and frankel defects, colour centres, non-stoichonmetry defects. Classification of solids, lattice energy, evaluation of madelung constant (NaCl), calculation of repulsive potential exponent. Lattice heat capacity, Einstein model and Debye model of lattice heat capacity, Debye T<sup>3</sup> law.

## Section-C

### **Polymer Chemistry**

Conducting polymers: conductive polymers *via* controlled pyrolysis, conduction mechanisms. Polyacetylenes (PA), polypyroles (PPY), polythiophenes (PT), polyparaphenylenes (PPP), polyparasulphide (PPS), polyanilines (PAN), organometallic conducting polymers and their applications.

### Section-D

### Introduction to Nanomaterials

Definition, historical perspective, consequences of nanoscale, nanoparticle morphology, lew methods of synthesis of nanomaterials and characterization techniques like XRD, SEM/TEM, scanning tunneling microscope (STM) and Atomic force microscopy (AFM).

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### Suggested readings

- 1. Modern electrochemistry Vol. 1 & II. JOM Bockris& Reddy.
- 2. Principles of electrochemisto 1 A Michnen.
- 3. Statistical thermodynamics. 1 : Hill. Addison Wisley, 1960.
- 4. Statistical thermodynamics, J. L. Wall, W. H. Freeman and Co., 1965.
- 5. Conducting polymer-Molecular recognization, advances in polymer science. Springer Verloag, New York.
- 6. Special polymers for electrome & optoelectrome and edited by J.A. Chilton & Goosey. Chapman Hall.

7. Physical chemistry a molecutar approach, Donald A. Macquirrie, John D. Simon, Viva Books Ltd., Ansari Road, N. Doshi

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