Course work: The revised course work comprises of following four papers-

**Paper I: CHEM-DPH 101:** This compulsory paper comprises the Research Methodologies/Philosophy, Review of Research work etc.

**Paper II: CHEM-DPH 102:** This discipline specific optional paper will comprise advanced organic, physical and smart functional materials papers which will cover topics of chemistry which are essential for Ph.D. scholar during his research work.

**Paper III: CHEM-DPH 103:** This compulsory paper comprises the applied spectroscopic techniques employed for characterization of compounds.

**Paper IV: CHEM-DPH 104:** This compulsory paper comprises instrumental techniques and computer aided drug designing.

- **Duration of Course Work:** One Semester (6 Months)
- **Total Marks:** 16 Credits
- **Course work: (Paper I-IV):** 16 credits
- **Duration of Examination:** 12 Hrs. (3 hrs. for each theory papers)
  1. **Paper I (CHEM-DPH 101):** Research Methodology 4 credits
  2. **Paper II (CHEM-DPH 102):** Discipline Specific Optional paper
     - **OPTIONAL I: CHEM-DPH 102-01:** Advanced Organic Chemistry 4 credits
     - **OPTIONAL II: CHEM-DPH 102-02:** Advanced Physical Chemistry
     - **OPTIONAL III: CHEM-DPH 102-03:** Advanced functional materials
  3. **Paper III (CHEM-DPH 103):** Applied Spectroscopy 4 credits

Examination will be held at the end of the Semester comprising 70 % end term and 30 % internal evaluation process.
PAPER I: CHEM-DPH 101  
Research Methodology

**Unit I: Research Aptitude:** Types of research, steps of research, materials for research (paper, articles, workshop, seminar, conferences and symposium), process of research: formulation of objectives, hypothesis, research plan, methods of research (survey, observation, experimental work, interpretation of data and result). Review of an articles and preparation of report. Thesis writing: Its characteristics and format. Review of literature of the previous work, use of internet in research activity.

**Unit II:** Methods of Data Collection  
**Statistical analysis:** Mean, standard deviation, variance, correlation coefficient and $\chi^2$ test. Regression analysis (linear/ non-linear), absolute and relative errors.  
**Web Browsing for Research:** Usage of Webs as a tool for scientific literature survey. Usage of packages/ software.

**Unit III:** Standard Protocols for Validation of Methods  

**Unit IV:** Intellectual Property Right (IPR)  

PAPER II: CHEM-DPH 102  
*(OPTIONAL PAPER)*

**OPTION I: CHEM-DPH 102-01: Advanced Organic Chemistry**

**Unit I: Introduction to Medicinal Chemistry**  
Role of Medicinal Chemists, Medicines, Current trends in Drug discovery, Drug Discovery Pipeline, Clinical trials, Leads and analogues: desirable properties, Sources of leads and drugs. Procedures followed in drug design, Classification of drugs: on basis of pharmacological activity, chemical structure, and origin, Methods of administration of drugs. Pharmacokinetics and Pharmacodynamics properties of Drugs.

**Unit II: Drug Design and Action**  
Concepts of prodrugs, Drug receptor interactions, Receptors, and their properties, types of receptors, Drug-response relationship (Agonist and Antagonists), Tachyphylaxis, structure-activity relationship (SAR) factors affecting bioactivity, Isosterism and bio-isosterism, Theories of drug activity (Clark’s occupancy theory, The Rate theory, The two-state model,..
Unit III Synthetic Reagents

(a) Oxidations: Metal based and non-metal based oxidations of alcohols to carbonyls (aluminium, DMSO, hypervalent iodine and TEMPO based reagents), alkenes to epoxides alkenes to diols, Prevost reaction and Woodward modification. Ketones to ester/lactones.

(b) Reductions Catalytic hydrogenation (Heterogeneous: Palladium/Rhodium; Homogeneous: Wilkinson), Hydride transfer reagents (i) NaBH₄ triacetoxyborohydride, Luche reduction; LiAlH₄, DIBAL-H.

Unit IV Sustainable Organic Synthesis

Introduction to Principles and concepts of green chemistry, Approaches for green: synthesis/reaction: Green starting materials, Green solvents: Aqueous medium, Ionic liquids, Solvent free reactions, Super Critical Fluids, Flourous phase reactions; Non-conventional energy sources; Microwave and Ultrasound assisted reactions

Recommended books:
1. A Guide Book to Mechanism in Organic Chemistry (Orient-Longmens)-Peter Sykes
5. Stereochemistry by P. S. Kalsi (New Age International)
12. Reaction Mechanism in Organic Chemistry- S. M. Mukherji and S. P. Singh
   Introduction to Stereochemistry (Benjamin)- K. Mislow
15. Fundamentals in medicinal chemistry- G. Thomas. 2nd edition
16. Introduction to medical Chemistry, G. L. Patrick
17. Medicinal Chemistry- Ashutoshkar
18. Medicinal Chemistry- Sreeram and Yogeshwari
19. Medicinal Chemistry & Drug discovery- Burger (Volume 1-6)
20. Burger’s medicinal chemistry vol. 1to6

OPTION II: CHEM-DPH 102-02: Advanced Physical Chemistry

Part-I Advanced Surface Chemistry

Gibbs adsorption isotherm, estimation of surface area (BET equation), surface film of liquids (electro-kinetic phenomenon), catalytic activity at surfaces and their mechanism, Various adsorption isotherms models including two, three, four, and five parameters. Giles classification of Adsorption isotherms shapes. Activated carbon properties, adsorption capacity, iodine
number, molasses number, product density, mesh size ash content, IUPAC classification of macro-meso-and micro-porous materials (pore size distribution), and industrial applications of adsorption.

**Part-II- Colloids and Surface Phenomenon**

Surface active agents, Classification of Surface active agents, micellization, hydrophobic interaction, critical micelle concentration (CMC), Kraft temperature, factors affecting the CMC of surfactants, counterion binding to micelles, thermodynamics of micellezation, mass action method and phase separation model of micellezation, solubilization, micro emulsion, reverse micelles, surface films. Surface characterization: Surface area, surface acidity and basicity, XPS, UPS, AES, EXAFS, XRD, SEM etc.

**Part-III- Advance Electrochemistry**


**Part-IV-Ultrasoundics Sonochemistry**


**Recommended Books**

3. Modern Electrochemistry- K.N. Reddy
5. Physical Chemistry- P.W. Atkins
6. Physical Chemistry (Part IV) - K.L. Kapoor
7. Physical Chemistry-Br. Puri, Lr. Sharma, Madan S. Pathania
8. Physical Chemistry-G.K. Vemulapalli
11. Fundamentals of Molecular Spectroscopy- Colin N. Banwell
12. Surface Chemistry- A Goel
13. Introduction to Surface Chemistry & Catalysis- Gabor A. Somorjai
14. Electrochemistry– Philip H. Rieger
15. Chemical Kinetics and Catalysis– Richard Mishel
16. Chemical Kinetics– Keith J Laidler
17. Handbook of Ultrasonics and Sonochemistry- Muthupandian Ashokkumar, Springer Nature
19. Micelle-Yoshikiyo Mori
20. Sonochemistry-Kenneth S. Suslick

OPTION III: CHEM-DPH 102-03: Advanced functional materials

Unit I Introduction to nanomaterials
Nanomaterials, role of size in nanomaterials, nanoparticles, semiconducting nanoparticles, nanostructures, nanowires, nanoclusters. Physico-Chemical and biological routes for the synthesis of nanomaterials, Optical, electronic, magnetic and electrical properties; band-gap, catalysis, and electronic devices.

Unit II Characterization Techniques:
X-ray diffraction, electron (SEM & TEM) and optical microscope, UV-VIS-IR spectrophotometers, thermal, magnetic and electrical measurements. Lithographic techniques: AFM, E-beam and SEM.

Unit III: Polymers and carbon based nanostructures
Preparation and characterization of block copolymer based nanocomposites, nanoparticles polymer ensembles, Fullerenes, CNTs, graphenes; Properties: mechanical, optical and electrical, nanomaterials in drug-delivery.

Unit IV: Modified Biopolymers: Definition of biopolymers, classification, mechanism of action, influence of various factors on the function of biopolymers, Modified Biopolymers: methods for biopolymer modifications, Applications of biopolymers

PAPER III: CHEM-DPH 103

APPLIED SPECTROSCOPY

Unit I:


Unit II:
Mass spectrometry, Basic principles, instrumentation, soft and hard ionization techniques FAB, EI-MS, ESI and MALDI-MS, isotope abundance, nitrogen rule, molecular ion, fragmentation processes of organic molecules, McLafferty rearrangement, deduction of structure using mass spectral fragmentation.

Unit III
NMR spectroscopy-I
1H NMR: Instrumentation, Magnetic and non-magnetic nuclei, Larmor frequency, absorption of
radiofrequency, chemical shift and its measurement, factors influencing chemical shift, deshielding, anisotropic effect, spin-spin coupling, factors influencing coupling constant, AB, AX and ABX systems, simplification of second order spectrum, selective decoupling, NOE effects, restricted rotation (DMF, DMA), cyclohexane ring inversion, chemical shift reagents for stereochemical assignments.

**Unit IV**

**NMR spectroscopy-II**

a) Introduction to $^{13}$C NMR, Off-resonance coupled and decoupled and DEPT method, Multinuclear NMR of Si, F and P nuclei.

b) Interpretation of spectra of compounds based on UV-visible, IR, mass and NMR spectroscopy.

**Recommended Books:**

1. Instrumental Methods of analysis- Willard, Merrit, Deanand Settle.
4. Absorption spectroscopy of organic molecules- V. M. Parikh
5. Applications of spectroscopic techniques in Organic chemistry- P. S. Kalsi

**PAPER IV: CHEM-DPH 104**

**Unit I**

**Electrokinetic Phenomenon**

Electrokinetic Effects, Electrokinetic potential/Zeta potentials, Determination of zeta potential, influence of ions on electrokinetic phenomena, Electro-Osmosis, Streaming potential, Sedimentation potential. Theoretical and quantitative treatment of electrokinetic phenomena, Electrophoretic Mobility and Bound hydrogen ion.

**Unit II**

**Polarography and Voltametry**

Electrode polarization, Theories of overvoltage, Importance of overvoltage, Principle of polarography, variations of the conventional polarographic methods, Pulse Polarography, Oscillographic polarography, Tensammetry, AC polarography, square wave polarography, Anodic stripping and cyclic voltametry, Qualitative and quantitative application of polarography, Determination of stoichiometry and formation constants of complexes. Amperometric titrations and advantages.

**Unit III**

**COMPUTER AIDED DRUG DESIGN (CADD) I**

Role of CADD in drug discovery, Different CADD techniques and their applications, Various Strategies to design and develop new drug like molecules, Working with molecular modeling softwares to design new drug molecules, The in silico virtual screening protocols, Quantitative Structure Activity Relationships: development of QSAR: Physicochemical parameters and methods to calculate physicochemical parameters: Hammett equation and electronic parameters (sigma), lipophilicity effects and parameters (log P, pi -substituent constant), steric effects (Taft steric and MR parameters).
Unit IV
COMPUTER AIDED DRUG DESIGN (CADD) I I
Molecular Modeling and Docking: Molecular and Quantum Mechanics in drug design, Energy Minimization Methods: comparison between global minimum conformation and bioactive Conformation, Molecular docking and drug receptor interactions: Rigid docking, flexible docking and extra precision docking. Agents acting on enzymes such as DHFR, TSPO, choline esterase (AchE & BchE) etc, Prediction and analysis of ADMET properties of new molecules and its importance in drug design.

Recommended Books
7. Modern quantum chemistry, N.S. Ostlund and A. Szabo, McGraw Hill
10. Exploring chemistry with electron structure methods, J. B. Foresman and E. Frish, Gaussian Inc.
11. Semi-empirical MO theory, J. Pople and D. L. Beveridge

(Dr. Jawahar Lal)  (Dr. Preeti Gupta)  (Dr. Shailesh Kumar)  (Dr. Jyoti Pandey)
(Invitee)         (Member)                 (Invitee)         (Invitee)

(Dr. Anjani K. Tiwari)  (Prof. Gajanan Pandey)  (Prof. K.N. Singh)  (Prof. Kuldip Singh Dhindsa)
(Invitee)                 (Member)                (External Member)   (External Member)

(Prof. Kaman Singh)
Chairman, BPGS