Department of Chemistry
School of Physical and Chemical Sciences

Syllabus of Ph.D. Coursework in Chemistry

Central University of South Bihar
Gaya-Panchanpur Road, Gaya-824236

Department of Chemistry

The Department of Chemistry under the School of Physical and Chemical Sciences forms a key component of the university. The department is composed of dynamic faculty members, students and research scholars who are actively engaged in knowledge creation and dissemination at the frontiers of the Chemical Sciences. The discipline has an encompassing effect on the biological and physical sciences and therefore considered a central science. The department believes in interdisciplinary approach of learning and fosters a culture of excellence. Undergraduate and Post-graduate students of chemistry are nurtured and mentored well to compete at the national and international level (eg. selection for the summer research fellowships of National Academies of Sciences, award at National Science Film Festival, JAM, UGC-CSIR NET, GATE and more…). The masters (M.Sc.) and doctoral (Ph.D.) programmes were started in 2018 and 2019, respectively. Although the department is relatively younger, it is scaling new heights with every passing year. Many of the alumni are now well-placed in different research and academic institutions of repute. Knowledge and skills in chemistry play a crucial role in finding the solutions to most of the challenges (eg. energy, disease, environment) faced by the mankind today. We envisage producing globally competent chemists who can solve the pressing problems of the nation.

Ph.D. in Chemistry

The faculty members and students of the department are engaged in cutting edge research at the frontiers of science. The PhD programme was launched in 2019-20 to further strengthen and institutionalize the culture of research and innovation. The department follows an interdisciplinary approach and offers diverse areas of research which include nano-chemistry, materials chemistry, organic synthesis, medicinal chemistry, photochemistry, catalysis etc. To further encourage the interdisciplinary research, the department has established inter-institutional links and collaborations with renowned laboratories and universities. During the programme, students will acquire new skills while working on state-of-the-art instruments in the department. The ultimate aim of the programme is to produce globally competent chemists who can critically think and analyse a problem, and develop innovative scientific solutions. Equipped with sound knowledge and lab skills, the doctoral students would be able to address some of the biggest scientific challenges facing the mankind today such as energy crisis, lighting & displays, sanitation, diagnostics & therapeutics and many more. The successful completion of the Ph.D. programme will ensure enhanced employability and the students are likely to get positions of eminence in leading research and academic institutions in India as well as abroad.

Laboratory Facilities & Resources

There are two laboratories in the department. Each lab is spacious enough to accommodate 40 students at a time. There are six working platforms (island tables) and four fumehoods fitted with inlet & outlets for water, LPG and nitrogen to perform the experiments. The lab is equipped with the sophisticated instruments, glassware, plasticware, chemicals & other lab peripherals. The sophisticated instruments available in the labs are as follows

- UV-Visible absorption spectrophotometer
- UV-Vis-NIR absorption spectrophotometer
- FTIR Spectrometer
- Luminescence Spectrometer
- Raman Spectrometer
- Particle Size Analyzer-cum-Zeta potential Measurement system (Dynamic Light Scattering set-up)

- Microwave Synthesizer
- Electrochemical Workstation
- Flash Chromatography
- Liquid Chromatograph -Mass Spectrometer (LCMS)
- Gas Chromatograph -Mass Spectrometer (GCMS)
- Digital pH Mater
- Digital Conductivity meter,
- Digital Thermometer
- Ultrasonicator
- Ice-Flaker
- Magnetic Stirrer cum hot plate (ceramic top)
- Incubator & Shaker
- Circulating water bath with temperature control (5^{o}C to 80 ^{o}C)
- Muffle Furnace

Eligibility Criteria for Admission to Ph.D. Programme

(A) Candidates for admission to the Ph.D. Programme in Chemistry shall have a Master's degree Chemistry/applied Chemistry or in allied subjects (including biochemistry, medicinal chemistry, industrial chemistry, nanoscience, environmental science) with at least 55% marks in aggregate or its equivalent grade 'B' in the UGC 7-point scale (or an equivalent grade in a point scale wherever grading system is followed) or an equivalent degree from a foreign educational Institution accredited by an Assessment and Accreditation Agency which is approved, recognized or authorized by an authority, established or incorporated under a law in its home country or any other statutory authority in that country for the purpose of assessing, accrediting or assuring quality and standards of educational institutions.

(B) A relaxation of 5% of marks, from 55% to 50%, or an equivalent relaxation of grade, may be allowed for those belonging to SC/ST/OBC (non-creamy layer)/Differently-Abled and other categories of candidates as per the decision of the Commission from time to time, or for those who had obtained their Master's degree prior to 19th September, 1991. The eligibility marks of 55% (or an equivalent grade in a point scale wherever grading system is followed) and the relaxation of 5% to the categories mentioned above are permissible based only on the qualifying marks without including the grace mark procedures.

(C) Subject to the conditions stipulated in these Regulations, the following persons are eligible to seek admission to the Ph.D. programme:
a) Master's Degree holders satisfying the criteria stipulated under Clause (A) and (B) above.
b) Candidates possessing a Degree considered equivalent to M.Phil. Degree of an Indian Institution, from a Foreign Educational Institution accredited by an Assessment and Accreditation Agency which is approved, recognized or authorized by an authority, established or incorporated under a law in its home country or any other statutory authority in that country for the purpose of assessing, accrediting or assuring quality and standards of educational institutions, shall be eligible for admission to Ph.D. programme.

MODE OF ADMISSION

A candidate who has passed the qualifying examination with requisite percentage of marks is eligible for admission to the Ph. D. Programme through one of the following modes:
(A) Admission through Entrance Test

(B) Direct Admission

COURSE WORK

- A candidate, admitted to the Ph.D. Programme in Chemistry, shall be required to undertake Course Work as approved by the Academic Council during the initial one or two semesters for a minimum period of one semester. However, this period may be extended for another semester as per the requirements of Department. The candidate shall have to qualify as per the criteria prescribed by the Course Work Ordinances of the concerned Department. The Course Work shall include a course on Research Methodology and Reviewing of Published Research Work in the relevant field.
- Candidates already holding M.Phil. Degree and admitted to the Ph.D. Programme, or those who have already completed the Course work in M.Phil. and have been permitted to proceed to the Ph.D. in Integrated Course, may be exempted by the DRDC/CRDC from the Course Work, subject to the fulfilment of the minimum credits requirement prescribed by the Department. Such candidates shall be issued an Exemption Certificate by the University. All other candidates admitted to the Ph.D. programme shall be required to complete the Ph.D. Course work prescribed by the Department.
- The credit assigned to the Ph.D. course work shall be a minimum of 08 credits and a maximum of 16 credits. A minimum of four credits shall be assigned to one or more courses on Research Methodology. Other courses shall be advanced level courses preparing the students for Ph.D. degree. The details of the courses, course credits and other related matters shall be determined in accordance with the Ordinances of the Department**.** However, a minimum of 75 % attendance shall be required in the Course Work for the research scholars registered on part-time basis.
- The Department where the scholar pursues his/her research shall prescribe the course(s) to him/her based on the recommendations of the Research Advisory Committee.
- The courses offered for the Ph. D. Programme may be through lecture, laboratory, field study, design and self-study courses, mini projects and seminars. Each of these courses shall be of doctoral level.

Course Structure of Ph.D. Programme

(Minimum Credits = 14)

Semester-I					
	Course Code	**Course Title**	**Theory/Practical(Hrs/Week)**	**Total Marks**	**Credit**
Core	CHE101DC00104	Research Methodology	4	100	4
Core	CHE101DC00204	Tools, Techniques and CurrentResearch Trends in Chemistry	4	100	4
Core	CHE101DC00302/ CHE101OE00102	Research and Publication Ethics	2	50	2
Semester-II					
Core	CHE102DC00104	Research Proposal Preparation and Seminar Presentation	4	100	4

Course Title: Research Methodology
Course code: CHE101DC00104

Course objectives: This course is designed to provide an overview on fundamentals of doing research including scientific terminology, literature, methods, analysis and interpretation of data, preparation of research report and presentation, future aspects of research as a career, importance and applications of scientific research to the society. It will help the students to develop core research skills relevant to a wide spectrum of chemical research including written and oral communication, skills in making scientific observations, and recording and analysing data by participating in discussions or through presentations or group research project associated with a discipline of interest to them. Assignments and tutorials would be included to enhance the course deliver and outcome.

UNIT I: Principles of Research (20H)

Foundation of Research: Objectives of scientific research, research & theory-conceptual and theoretical model, importance of research methodology in scientific research, types and methods of research, evaluation of research/study.
Research problem: meaning of research problems, sources of research problems, criteria/ characteristics of a good research problem, errors in selecting a research problem. Hypothesis: Meaning, types of hypothesis.
Design and execution of experiments, collection and interpretation of experimental data, arriving at conclusions.
Errors in chemical analysis, classification of errors, determination of accuracy of methods, improving accuracy of analysis, significant figures, mean, standard deviation.
Basic knowledge of computer systems: General awareness of software packages and other scientific applications. Knowledge of MS office application, spreadsheets, basic ideas on the use of internet in chemistry education. Knowledge of data analysis for research publications.

UNIT II: Literature Survey (15H)

Introductions: Sources of information, need for reviewing literature, primary-secondary and tertiary sources, journals, journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text books, current contents, patents. Introduction to chemical abstracts and beilstein, subject index, substance index, author index, formula index and other indices with examples.
Digital: Web resources, E-journals, journal access, TOC alerts. Hot articles: Citation index, UGC infonet, E-books, Impact Factors, Search engines- Google scholar, chemical industry, Wiki-databases, chemSpider, ScienceDirect, SciFinder, Scopus.

UNIT III: Concepts of Chemical Safety (15H)

Chemical safety and ethical handling of chemicals, safe working procedure and protective environment, emergency procedure and first aid, laboratory ventilation, safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmosphere, safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals.

UNIT IV: Ethics and IPR (10H)

Regulatory bodies, practices and compliances, Good Laboratory Practices (GLP), Research Ethics & Misconduct, Patents, Copyrights, GI and Trademarks, Product and process patent, Patent Treaties and Convention, process of filing patent, database of patent, search and retrieval.

References

1. Practical Skills in Chemistry, J. R. Dean, A. M. Jones, D. Holmes, R. Reed, J. Weyers and A Jones, Pearson Education Ltd., Prentice Hall, (2002).
2. Research Methodology. Methods and Techniques: C. R. Kothari.
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4. Robert V Smith, Graduate Research: A Guide for Students in the Sciences, University of Washington Press, 1998.
5. Biggs Pete, Computers in Chemistry, Oxford University Press, 2000.
6. Cropper William H, Mathematical Computer Programs for Physical Chemistry, Springer.
7. Chemical Safety Manual, IIT Bombay. http://www.iitb.ac.in/safety/sites/default/files/chemical%20safety%20manual.pdf.
8. Chemical Safety Manual, ACS. https://www.acs.org/content/dam/acsorg/about/governance/committees/chemicalsafety/publications/chemical-safety-manual-teachers.pdf.

Course Title: Tools, Techniques and Current Research Trends in Chemistry *(Any Four Units to be covered, Unit I or Unit II are compulsory)*

Course Code: CHE101DC00204

Course Objectives: The objectives are

1. To impart necessary skills in spectroscopy techniques such as NMR, fluorescence and mass spectrometry
2. To make students learn the imaging techniques such as SEM, TEM, AFM and STM.
3. To make students aware of the latest research trends in the area of their interest

UNIT I: Spectroscopy and Spectrometry (24H)

NMR Spectroscopy: NMR phenomenon, spin ½ nuclei, Zeeman splitting, effect of magnetic field strength on sensitivity and resolution, chemical shift □, inductive and anisotropic effects on □, chemical structure correlations of □, chemical and magnetic equivalence of spins, spin-spin coupling, structural correlation to coupling constant J, first order patterns. Second order effects, selective decoupling, use of chemical shift reagents for stereochemical assignments. 1H and 13C chemical shifts to structure correlations. Study of dynamic processes by NMR. 2D NMR and its application in organic chemistry

UV-Vis and IR: Principles and applications
Fluorescence Spectroscopy: Introduction, Phenomenon and characteristic of fluorescence, fluorescence life time, Fluorescence Resonance Energy Fluorescence quenching, types of quenching processes, Transfer Instrumentations, experiments for fluorescence quenching measurements, Applications of Fluorescence Spectroscopy.
Mass Spectrometry: Introduction and its application

Unit II: Imaging and Microscopy (24H)

Scanning Electron Microscope (SEM): SEM Basics of electron optics, resolution in SEM. Contrast Mechanisms. Detectors. STEM. Sample preparation for the SEM.
Atomic Force Microscopy (AFM): Basic Machinery, Deflection detection methods, control systems. Harmonic oscillator response. Contact mode AFM. Lateral Force Microscopy. Determination of spring constants,
Scanning Tunneling Microscopy (STM): Theoretical Description of tip-sample tunnelling. STM components. Feedback control. Speed. Stability and Drifts. Vacuum and Low temperature STM. Application examples, Scanning Tunneling Spectroscopy and Spectroscopic Imaging. Interpretation of STM data;
Transmission Electron Microscopy (TEM): Theoretical Description of TEM image formation. Anatomy of the TEM. Sample preparation.

Unit III: Nanomaterials (12H)

Introduction to the nano- the length scale, meaning of the terms nanomaterials, nanoscience and nanotechnology Nanomaterials as low dimensional systems, classification into 2D, 1D and 0D systems. Electronic structure of such systems
Stabilization of colloidal nanoparticles, electrostatic and steric stabilization, surface functionalization of nanoparticles. Classification of nanomaterials
Nanocomposites: Different types of Nanocomposite; Core-Shell structured nanocomposites; Superhard Nanocomposites
Synthesis of nanomaterials: Top-down, bottom-up approach, liquid-phase synthesis, gas-phase synthesis, vapour-phase synthesis

Unit IV: Supramolecular Chemistry (12H)

Terminologies and nomenclature in supramolecular chemistry, Chemical interactions leading to supramolecular assemblies; Molecular recognition through pre-organisation and complementarity. Concept of molecular receptors and design principles. Receptors and coordination and inverse coordination, host-guest chemistry, synthesis of supramolecular structures.
Molecular machines, molecular and supramolecular devices, supramolecular photochemistry and photonic devices, Molecular wires and rectifying devices. Ion responsive monolayers, application of supramolecular chemistry.

Unit V: Bio-inorganic Chemistry (12H)

Metal ions in biology; Active-site structure and function of metallo-proteins and enzymes with Mg, Ca, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Mo and W ions.
Heme and Nonheme structures with mono-, di- and multinuclear metal centers, such as Fe: Hb, Mb, Hr, P-450, MMO, ferridoxins, Fe-S clusters; Cu: hemocyanin, hemerythrin; Mn: SOD, Catalase; Co: vitamin B12; Zn, Ni, urease. Metal environments (ligand type, coordination, geometry), electronic, magnetic and redox properties. Use in biological processes. Additional discussions on Nitrogenase and Oxygen Evolving Centre in Photosystem II.

Unit VI: Sustainable Energy Source (12H)

Introduction to hydrogen as a Green Fuel. Current energy Scenario, fuel, present, past and future. Hydrogen as a chemical fuel, the hydrogen economy, hydrogen production.
Concepts in photochemical water splitting, hydrogen production by water splitting. Recent trends in water splitting.
Solar cells: Principles for conversion of solar energy to electricity, fundamental calculations and measurement of efficiency of solar cells, different solar cell techniques, photoelectric energy, dye sensitized solar cells, charge separation and transport, new solar cell materials.

Unit VII: C-H activation and C-C coupling (12H)

Introduction, History of C-H activation and C-C coupling reactions, brief comparisons of chemistry of different metal mediated reactions, Pd(II)-Catalyzed C–H Activation/C–C cross-coupling reactions, catalytic cycle, olefination of sp^2 C–H bonds, arylation of sp^2 and sp^3 C–H bonds. Palladium-catalyzed carbon-carbon bond formation via cross coupling

Unit VIII: Fluorine Chemistry (12H)

Introduction of organofluoro compounds, Properties of fluorine atom, Effects of fluorine in organic compounds, Electrophilic and nucleophilic fluorinating agents and their application in organic synthesis, medicinal chemistry and agrochemistry. Organic synthesis of fluoroorganic compounds directed by use of organomettalic reagent and free radical fluorination

Unit IX: Organocatalysis (12H)

General Principles: Energetic, Catalytic cycles, catalytic efficiency and life time, selectivity.
Introduction of organocatalysis, activation mode, importance and clssifications, examples by taking C-C bond formation reactions, asymmetric synthesis by organocatalysis

Unit X: Green and Sustainable Organic Synthesis (12H)

Sustainable Organic Chemistry, catalyst, Introduction to Green Chemistry, Green Solvents:

Water, ionic liquids, supercritical fluids, glycerol, biphasic systems, eutectic solvents. Radiation based techniques in green synthesis: microwave synthesis, and sonochemical based synthesis.

Unit XI: Medicine from Natural Products (12H)

Natural Products, Metabolites, Drug, medicine and poison, Traditional medicine, drugs developed from natural products, drugs developed from traditional medicine, Case studies of development of drug for malaria and antibiotics. Nature as a source of inspiration for development of new drugs. Techniques of Isolation: extraction, separations, and characterisation

UNIT XII: Computational Chemistry (12H)

List useful numerical methods for chemistry. Potential energy surfaces and intermolecular interactions: Quantum mechanical ab initio calculations. Energy calculations using molecular mechanics. Approximation of the total potential energy. Study of cluster and bulk properties through simulations. Modelling of small molecules. Nonpolarizable and polarizable rigid models. Flexible models and calculation of force constants. Structural, dielectric and dynamical properties of a polar medium: Continuum models versus molecular models.

UNIT XIII: Polymers (12H)

Conducting polymers: Electrically conducting polymers and their uses (polyanilines, polypyrrole, polyacetylene and polythiophene). Photoconductive polymers. Liquid crystal polymers – smectic, nematic and cholesteric structures. **Ionic exchange polymers***:* Cationic and anionic exchange polymers and their uses. Eco-friendly polymers. Poly lactide from corn derived dextrose, PHB etc. Membrane separation. Filtration – micro, ultra and nanofiltration. Separation of gases – permeselectivity and gas permeability of representative polymers. Liquid separation – dialysis, electro osmosis and reverse osmosis. Fire retarding polymers, photonic polymers. Inter penetrating networks (IPN), polymers in photo lithography.

UNIT XIV: Biophysical and Surface Phenomena (12H)

Biophysical Chemistry and Surface Chemistry: Thermodynamics in Biochemistry (Fundamentals and Applications); Biopolymers; Biomembranes, Active transport and passive transport, Multiple equilibria, Specific examples of multiple equilibria, Transport processes; General features of transport processes; Optical systems for the study of transport processes, self organizing systems their interactions and solutions properties. Preparation, Characterization and Application of nanoparticles Surface and Biophysical Techniques.

UNIT XV: Electrochemical Techniques and energy conversions (12H)

Electrochemical processes and techniques:
Electrical double layers, surface tension and electrocapillarity. Kinetics of multistep charge-transfer reactions. Mass transfer. Electrochemical methods: Voltammetry, chronoamperometry, chronopotentiometry, electrochemical impedance measurements, Electrocatalysis, Spectroelectrochemistry and scanning-probe methods, Electrochemical quartz balances, Nucleation and electrocrystallization

Electrochemical Energy Conversion:

Supercapacitors: porous 3D-electrodes, charge-discharge cycles, redox supercapacitors based on MnOx and RuOx redox processes; ***Primary batteries:*** batteries based on zinc-manganese, zinc-air and lithium-ion chemistry; ***Secondary batteries:*** rechargeable systems, lead-acid battery, lithium ion battery and their functioning; ***Fuel cells and flow batteries***: Polymer electrolyte fuel cell, Solid oxide fuel cells , Vanadium flow batter; ***Electrolyzers:*** KOH electrolyte based alkaline electrolyzer, acidic polymer electrolyte membrane electrolyzers

References

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Sustainable Energy Source:

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2. Green Chemistry: An Introductory Text by Mike Lancaster, Royal Society of Chemistry, 2nd edition 2010.
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Course title: RESEARCH AND PUBLICATION ETHICS

Course Code: CHE101DC00302/CHE101OE00102

Course Objectives: The objectives are

1. to make the students aware about the fake journals and predatory publishers
2. to inculcate robust research culture devoid of unethical practices.
3. to impart the necessary skills of scientific literature search through different databases and search engines

THEORY

UNIT 1: PHILOSOPHY AND ETHICS (3 HRS)

1. Introduction to philosophy: definition, nature and scope, concept, branches
2. Ethics: definition, moral philosophy, nature of moral judgements and reactions.

UNIT 2: SCIENTIFIC CONDUCT (5 HRS)

1. Ethics with respect to science and research
2. Intellectual honest and research integrity
3. Scientific misconducts: falsification, fabrication, and plagiarism.
4. Redundant publications: duplicate and overlapping publications, salami slicing
5. Selective reporting and misrepresentation of data.

UNIT 3: PUBLICATION ETHICS (7 HRS)

1. Publication ethics: definition, introduction and importance
2. Best practices/standards setting initiatives and guidelines: COPE, WAME, etc.
3. Conflicts of interest
4. Publication misconduct: definition, concept, problems that lead to unethical behavior andvice verse, types
5. Violation of publication ethics, authorship and contributor ship
6. Identification of publication misconduct, complaints and appeals
7. Predatory publishers and journals

PRACTICE

UNIT 4: OPEN ACCESS PUBLISHING (4 HRS)

1. Open access publications and initiatives
2. SHERPA/RoMEO online resource to check publisher copyright and self-archivingpolicies.
3. Software tool to identify predatory publications developed by SPPU
4. Journal finder/ journal suggestion tools viz. JANE, Elsevier Journal Finder, SpringerJournal Suggested, etc.

Unit 5: PUBLICATION MISCONDUCT (4 HRS)

A. Group Discussions (2 hrs)

1. Subject specific ethical issues, FFP, authorship
2. Conflicts of interest
3. Complaints and appeals: examples and fraud from India and abroad

B. Software tools (2 hrs): Use of plagiarism software like Turnitin, Urkund and other opensource software tools.

Unit 6: DATABASES AND RESEARCH METRICS (7 HRS)

A Databases (4 hrs)

1. Indexing databases
2. Citation databases: Web of Science, Scopus, etc.

B. Research Metrics (3 hrs)

Impact Factor of journal as per journal citation report, SNIP, SJR, IPP, Cite Score. Metrics: h-index, g index, i10 index, altmetrics

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7. Resnik, D.B. (2011). *What is Ethics in Research & Why is it Important.* National Institute of Environmental Health Sciences, 1-10. Retrieved from https://www.niehs.nih.gov/research/resources/bioethics/whatis/index.cfm

Course Title: Research Proposal Preparation and Seminar Presentation

Course Code: CHE102DC00104

Course Objectives: The objectives are

1. To make students proficient in chemistry-specific software
2. To make students learn how to conduct literature survey and design a research proposal

UNIT I: Research Proposal (15H)

Developing a Research Proposal: Format of research proposal, individual research proposal and institutional proposal. Research Report: Format of the research report, style of writing the report, references and bibliography

Application and uses of common software in chemistry- origin, chemsketch, chemdraw. Gaussian software and its use.

UNIT II: Literature Survey (45H)

Extensive survey of published literature relevant to the chosen topic of research which appeared in referred research journals of national and international repute, edited books, reference books, monographs, survey / study reports, dissertations / theses published in book form, and books / reports containing proceedings of national and international conferences / seminars / symposia. Students have to make a review on the given topic/proposal of research work.

There will be two seminar presentations (*viz.* presentation-I and presentation-II). The Ph.D. seminar courses require students to attend and deliver seminars as per their selected themes. Evaluation will be based on review preparation, participation and on the quality of the talk delivered.