Department of Chemistry
School of Physical and Chemical Sciences

Syllabus of Ph.D. Programme in Chemistry

(Proposed to be implemented from the session 2019-2020)

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 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. Knowledge and skills in chemistry play a crucial role in finding the solutions to most of the challenges (eg. energy, disease, and environment) faced by the mankind today. The department believes in interdisciplinary approach of learning and fosters a culture of excellence. Undergraduate students of chemistry have been nurtured and mentored well to compete at the national and international levels (eg. selection for the summer research fellowships of National Academies of Sciences, award at National Science Film Festival and more…). The postgraduate programme was launched from the last academic session in 2018-19. Going stronger with the research component, Ph.D. programme is being started from this new academic session in 2019-20. The department envisages scaling greater heights with the launch of Ph.D. programmes and producing globally competent chemists who can solve the pressing problems of the nation.

MSc. in Chemistry

The programme is for the students who have an interest in chemistry and a desire to explore the frontiers of science. This is a unique programme that combines core chemistry (Organic, Inorganic and Physical) with Nano Chemistry and Green Chemistry. Along with thorough grounding in chemistry, it equips the students with the knowledge and skills in the emerging interdisciplinary area of green nanotechnology which has now become a crucial requirement for the sustainable development globally. Computational Chemistry and Medicinal Chemistry have also been incorporated to equip the students better. The programme follows choice-based credit system (**CBCS**) where students have the liberty to choose courses from the elective baskets of our department or other departments. The students also have the freedom to choose a few online courses through **SWAYAM** (Study Webs of Active – Learning for Young Aspiring Minds) portal which further enhances learning. The programme envisages creating good bench strength of future scientists who can solve a wide range of issues and contribute to the scientific advancement of the nation. There is ample opportunity and employability of chemists having sound knowledge, analytical skills and hand-on training on the sophisticated instruments. The chemical industry is India's one of the largest manufacturing sectors and plays an integral role in the country's economic development. The Indian chemical sector currently accounts for 13-14% of total exports. In terms of volume of production, it is the twelfth-largest in the world and the third-largest in Asia. Currently, the per capita consumption of products of the Indian chemical industry is one tenth of the world average, which reflects the huge potential for further growth. The "Make in India" scheme has further given a fresh impetus to this sector. For a sustainable, environment friendly growth, the sector is looking for new technologies that incorporate green chemistry and nanotechnology and there lies the exciting and excellent career opportunities for young chemists. Besides chemical industry, the training imparted in the interdisciplinary area of green nanotechnology will also enable the students to diversify and join other sectors such as energy, photovoltaics, photonics, biosensing and healthcare etc. The curriculum has been designed to keep abreast with changing times. In the long run, the programme is likely to produce globally competent chemists with bright innovative ideas. By

understanding the nuances of chemistry, these young scientists would be creating new tools, products and technologies to address some of the world's biggest challenges such as (just to name a few) clean affordable energy, biomedical devices and drugs for treating diseases, biosensing and environmental remediation etc.

Ph.D. in Chemistry

The faculty members and students of the department are engaged in cutting edge research at the frontiers of science. The launch of Ph.D. programme in the upcoming academic session in 2019-20 will 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
- 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)

FTIR and Luminescence spectrometers are in advanced stages of procurement and are likely to be installed in the upcoming session 2019-20.

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 Core = 12)

		Course Title	Theory/Practical (Hrs/Week)	Total Marks	Credit
Core	CHE901	Research Methodology	4	100	4
Core	CHE902	Tools, Techniques and Current Research Trends in Chemistry	4	100	4
Core	CHE903	Research Proposal Preparation and Seminar Presentation	4	100	4

Research Methodology

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.

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Tools, Techniques and Current Research Trends in Chemistry

(Any Four Topics will be covered, Unit I or Unit II are compulsory)

UNIT I: Spectroscopy and Spectrometry (24H)

NMR phenomenon, spin ½ nuclei, Zeeman splitting, effect of magnetic field strength on sensitivity and resolution, chemical shift δ, inductive and anisotropic effects on δ, chemical structure correlations of δ, 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. ^{1}H and ^{13}C 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.

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Research Proposal Preparation and Seminar Presentation

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 softwares 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 deliver.