

**Learning Outcome Based Curriculum
Framework (LOCF)**

for

(Ph.D. Course Work in Chemistry)



(Effective from the Academic Year 2020-21)

Prepared by

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PREFACE

In compliance with the Rajiv Gandhi University guidelines for adaptation of Choice Based Credit System (CBCS) vide letter no. AC-845/PhD.Ent/08(Vol-III)/918 dated 02/03/2021, Department of Chemistry prepared the syllabus for the course work for Doctor of Philosophy (Ph.D.) in Chemistry to be effective from the academic session 2020-21.

The Syllabus framed by the Board of Post Graduate Studies (BPGS) for the Ph.D. Course Work as per CBCS format is presented herein. The syllabus was drafted as per the UGC guidelines for Learning Outcomes based Curriculum Framework (LOCF) based approach. Focus has been given to inculcate interdisciplinary skills that would allow the students in their proposed research work plan.

Students admitted under Ph.D. program will have to undergo a compulsory course of 6 (six) months duration of 12 credits. Detailed distribution of courses and the corresponding credits are given subsequently. Students are allowed to choose elective courses in different fields of chemistry. Current course is in line with the vision of RGU for providing a rigorous academic curriculum and a vibrant atmosphere for learning that equips students to solve national and global concerns. These are evident in the emphasis in all courses on fundamentals and on flexibility, in the incorporation of regional, national and global components in the learning objectives.

Rono Hills, Doimukh

Dr. Rajesh Chakrabarty
Chairman
Board of Post Graduate Studies (BPGS)
Department of Chemistry, RGU

DEPARTMENTAL PROFILE

The Department of Chemistry was established in the year 2011. It marked a humble beginning to impart quality teaching in chemistry and research in frontier areas of chemistry in this region of India. Department of Chemistry, situated in the lush green surroundings on the University Campus, offers programs leading to M.Sc. and Ph.D. degrees.

The Department offers a Two-year M.Sc. programme with specialization in all major areas of chemistry to provide students with the necessary theoretical background and introduction to laboratory methods. In addition to providing a rigorous academic curriculum and a vibrant atmosphere for learning basic and applied chemistry, we aim to produce high-quality graduates who can prove themselves in addressing the challenges in chemistry through research and innovation.

Department is striving to mark its footprint in the diverse areas modern chemical research via its well-trained young faculties. The Department is offering Ph.D. programme in chemistry since 2014. The region being a biodiversity hotspot, there is an immense potential for research and development in the field of natural products and medicinal chemistry. In this regard, we are engaged in sustainably harnessing the vast natural resources and endemic medicinal plants of this region to improve the quality of life of the citizens of the country. The faculties are actively involved in research via sponsored research projects. Since its inception, faculties have been able to receive support for their research projects from various funding agencies – DST (Department of Science & Technology), DBT (Department of Biotechnology), CSIR (Council for Scientific and Industrial Research), UGC (University Grants Commission) and UGC-DAE-Consortium for Scientific Research.

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REGULATIONS RELATING TO Ph.D. COURSE WORK

(As per the DOCTOR OF PHILOSOPHY (Ph.D.) ORDINANCE, 2020 of Rajiv Gandhi University)

- (a) The credit assigned to the Ph.D. course work shall be a minimum of 8 (eight) credits and a maximum of 16 (sixteen) credits.
- (b) The course work shall be treated as prerequisite for Ph.D. preparation. The Department/Institute/Centre shall assign a minimum of four credits to one or more courses on Research Methodology covering areas such as quantitative methods, computer applications, review of published research in the relevant field, training, field work, etc. Additionally, there shall be a compulsory course paper of two credits on Research and Publication ethics (as per the directives of UGC vide DO no-F.I-1/2018(Journal/CARE) dated December 2019). Other courses, with rest of the credit, shall be advanced level courses preparing the students for Ph.D. degree.
- (c) The course work for Ph.D. shall be prescribed by the BPGS of the concerned Department/ Institute/ Centre and approved by the FBS and the AC. All courses prescribed for Ph.D. course work shall be in conformity with the credit hour instructional requirement and shall specify content, instructional and assessment methods. The concerned DBS shall slightly modify/upgrade the contents of the course work as and when required and implement the same from next academic session on approval by the FBS and the AC.
- (d) The Department where the scholar pursues his/her research shall prescribe the course(s) to him/her based on the recommendations of the RAC and approved by the DRC.
- (e) Admitted scholars shall be required to complete the prescribed course work during the initial one semester as a regular student fulfilling the mandatory attendance and other associated requirements for successful completion of the course. In-service candidates admitted in the Ph.D. course shall have to take mandatory study leave for the period from their employer/competent authority. However, those scholars who have been awarded M.Phil. Degree and/or have successfully passed M.Phil./Ph.D. course work in the concerned/relevant subject/discipline shall be either fully or partially exempted as the case may be from doing the prescribed course work provided such course work pursued earlier by them is considered equivalent and appropriate by the RAC and DBS, and so approved by the competent authority of the University. Such scholars as have been prescribed to pursue additional course work paper(s) shall have to fulfil the minimum requirement of 8 (eight) Credits to complete the course work.
- (f) The course work shall be evaluated on the basis of the performance of the scholar in the Internal assessment examination(s) to be conducted by the concerned Department/ Institute/Centre, and the End semester examination to be conducted by the University. The weightage for the Internal assessment and the End semester examination shall be in 25:75 ratio. In case, the scholar fails to secure a minimum of 55 % marks in the Internal assessment examination, he/she shall be dropped from the programme.
- (g) A scholar has to obtain a minimum of 55 % of marks or its equivalent grade in the UGC 7- point scale (or an equivalent grade/CGPA in a point scale wherever grading system is followed) in the course work in order to be eligible to continue in the programme and submit the thesis. In case the scholar fails in the End Semester Examination of the course work, a supplementary examination shall be conducted by

the University within two months from the date of declaration of the result. However, the scholar shall be dropped from the program if he/she fails again to clear the examination.

1. TYPES OF COURSES

Usually a course refers to a 'paper' and is a component of an academic programme. Courses in Ph.D. course work shall be of two kinds: **Core** and **Elective**.

- (a) **Core Courses:** A core course is a compulsory paper to be studied by all the scholars to complete the requirements of the Ph.D. degree.
- (i) A course of 4 (four) credits on Research Methodology covering areas such as quantitative methods, computer applications, review of published research in the relevant field, training, field work, etc.
 - (ii) Research and Publication Ethics: The department shall offer a course paper of 2 (two) credits on Research and Publication ethics (as per the directives of UGC vide DO no - F.1- 1/2018(Journal/CARE) dated December 2019).
- (b) **Elective Courses:** Elective course is a course which can be chosen from a pool of papers from a syllabus provided by a particular department from the main discipline or from a sister/related discipline which supports the main discipline, on mutual consent of the concerned departments.
- (i) **Open Elective:** These courses shall constitute a pool of open elective courses. These courses offered by a department shall serve as open elective for other department(s).
 - (ii) **Discipline Specific Elective (DSE):** It shall be supportive to the discipline of study, providing an expanded scope, enabling an exposure to some other discipline/domain, and nurturing research scholar's proficiency/skill.
 - (iii) **Massive Open Online Course (MOOC):** Scholars can opt relevant courses from SWAYAM platform having minimum of 4 Credit course as per the recommendation of RAC.

2. COURSE CODING

- (a) The courses offered by the department carry a three-letter departmental code (CHE) that is followed by a single-letter code like; **C** for Core, **E** for Discipline Specific Elective and **O** for Open Elective. Next three-digit number refers to course code series; **6XX**.
- (b) The number of credits is given in the form **L:T:P**, where **L** indicates the number of contact hours of lecture, and **T** the number of contact hours for tutorials, **P** stands for laboratory credits and **C** for total credit per course. Each lecture credit corresponds to one lecture hour per week, while each laboratory credit corresponds to a 2-hour laboratory class. For example, 3:1:0 credits indicates that the course would have 3 lecture hours along with one tutorial session and no laboratory each week, while 1:0:1 credits indicates a course with one lecture hour, no tutorial session and one 2-hour laboratory.

3. GRADE POINT AND GRADE LETTER

- (a) Under the absolute grading system adopted by the University, the marks shall be converted to grades based on pre-determined class intervals. The grading system with the following letter grades shall be adopted in awarding the grades and CGPA under the credit-based semester system.

% of Marks	Grade Point	Grade Letter
≥ 90 but ≤ 100 %	10	O (Outstanding)
≥ 80 but ≤ 90 %	9	A (Excellent)
≥ 70 but ≤ 80 %	8	B (Very Good)
≥ 60 but ≤ 70 %	7	C (Good)
≥ 55 but ≤ 60 %	6	D (Average)
Below 55 %	0	F (Fail)
Absent	0	AB (Absent)

- (b) A Research Scholar obtaining Grade F shall be considered failed and shall be required to reappear in the examination.

4. COMPUTATION OF SGPA AND CGPA

- (a) The computation of the Semester Grade Point Average (SGPA) and Cumulative Grade Point Average (CGPA) shall be done as follows:
- (i) Semester Grade Point Average (SGPA) is the sum of the products of the course credit and grade points scored by a research scholar divided by the sum of all course credits offered by the research scholar. It can be calculated in the following manner:

$$SGPA (S_i) = \frac{\sum(C_i \times G_i)}{\sum C_i}$$

Where, C_i is the number of credits of the i^{th} course and G_i is the grade point scored by the research scholar in the i^{th} course.

- (i) Cumulative Grade Point Average (CGPA) is the sum of the products of the total number of credits of all courses taken by a research scholar in a semester with the SGPA in that semester divided by the total number of credits of all courses taken. It can be calculated in the following manner:

$$CGPA = \frac{\sum(C_i \times S_i)}{\sum C_i}$$

Where, S_i is the SGPA of the i^{th} semester and C_i is the number of credits in that semester.

COURSE STRUCTURE

- (a) The duration of the Ph.D. course work shall be of 1 Semester (6 months).
- (b) The credit assigned to the Ph.D. course work consisting of 4 (four) courses shall be a minimum of 12 credits and a maximum of 16 credits.
- (c) These 12 credits shall be distributed as follows:

Course Code	Course Title	Type of Course	Maximum Marks			Credit Distribution	Credit
			Internal Assessment	Terminal	Total	L : T : P	
CHE C 601	Research Methodology	Core	20	80	100	3:1:0	4
CHE C 602	Research and Publication Ethics	Core	25	25	50	1:0:1	2
CHE OE 61X	Open Elective <i>(Scholars shall have to opt any one course from the following list as per the recommendation of RAC)</i>	Elective I	10	40	50	2:0:0	2
	1. CHE OE 611: Spectroscopic Tools for Small Molecule Characterisation 2. CHE OE 612: Techniques for Material Characterization						
CHE DE 6XX	Discipline Specific Elective <i>(Scholars shall have to opt any one course from the following list as per the recommendation of RAC)</i>	Elective II	20	80	100	3:1:0	4
	1. CHE DE 621: Chemistry of Natural Products 2. CHE DE 622: Chemistry of Nanomaterials 3. CHE DE 623: X-Ray Crystallography for Chemists 4. CHE DE 63X: Massive Open Online Course (MOOC) <i>(Scholars can opt relevant courses from SWAYAM platform having minimum of 4 Credit course as per the recommendation of RAC)</i>						
			75	225	300		12

- (d) The open elective courses are of interdisciplinary nature and can be opted by the scholars from other departments. Scholars shall have to opt any one course from the list as per the recommendation of RAC.
- (e) Scholars shall have to opt any one course from the list as per the recommendation of RAC.
- (f) Discipline Specific Elective (DSE) courses provide an expanded scope, enabling an exposure to some other discipline/domain, and nurturing research scholar's proficiency/skill. Scholars shall have to opt any one course from the list as per the recommendation of RAC.
- (g) Scholars will also have the option to opt for Massive Open Online Course (MOOC) from SWAYAM platform having minimum of 4 Credit course as per the recommendation of RAC.

PROGRAM SPECIFIC OUTCOMES

- PSO 1:** To apply the fundamental knowledge of chemistry to seek solutions to complex problems in modern chemistry.
- PSO 2:** To integrate and apply relevant knowledge to problems that emerge from the broader interdisciplinary and multi-disciplinary areas such as life sciences, health & medicines, energy, materials, environmental sciences etc.
- PSO 3:** To develop skills to design and test hypothesis, execute research experiments, conduct chemical syntheses, analyses or other chemical investigations, compile raw data and provide conclusions.
- PSO 4:** Design solutions for complex scientific problems and develop innovative processes that meet the specified needs with appropriate consideration for the public health and safety, and the cultural, societal, and environmental considerations.
- PSO 5:** Apply ethical principles in research and commit to professional ethics, responsibilities and norms.
- PSO 6:** Independently explore new areas of research in both chemistry and allied fields of science and technology.
- PSO 7:** To inculcate skill in problem solving, critical thinking and reasoning vis-à-vis scientific problems.
- PSO 8:** Function effectively as an individual, and as a member or leader in diverse teams, and in multidisciplinary settings.
- PSO 9:** Communicate effectively on complex scientific results with the peers and with the society at large, such as, being able to comprehend and write effective reports and design documentation, make effective presentations, and give and receive clear instructions.
- PSO 10:** To have the preparation and ability to engage in independent and life-long learning in the context of scientific advance.

CHE C 601 Research Methodology

Total Credit Hours: 40
Credit: 4 (L 3 – T 1 – P 0)
Terminal Examination Duration: 3 Hours
Maximum Marks: **100** (Terminal – 80, Internal Assessment – 20)

Course objectives:

1. To help students in formulation of research aims and objectives in an appropriate manner.
2. To help the students in framing good research hypothesis.
3. To inculcate knowledge of scientific methodology in analysing research data.
4. To impart the knowledge of sampling techniques and record scientific data in a proper way.
5. To acquaint the students with chemistry related software and online scientific databases like Scifinder, Cambridge Structural Database (CSD) etc.

Learning Outcomes:

On completion of this course the students will be able to:

1. Understand the aims and objectives research and formulate a research work plan in a scientific manner.
2. Generate good research hypothesis, design appropriate experiments, collect and interpret the data to validate their experiments.
3. Process the data using computer software, analyze the data and critically examine the hypothesis and the conclusions.
4. Obtain and evaluate information from a variety of databases.
5. Communicate effectively in a variety of forms like research publications, patents, etc.

Introduction to Research Methodology (10 Hrs.): An introduction to basics of scientific research: objectives of research, types of research, research process and steps involved. Identification, selection and formulation of research problem. Intellectual property rights.

Sampling and Data Collection (10 Hrs.): Sampling: design and types; steps involved in sampling; sample size; advantages and limitations. Data types and collection: qualitative and quantitative, data processing, data analysis. Use of databases (SciFinder, Cambridge Structural Database, etc.).

Computational Methods for Data Analysis and Presentation (10 Hrs.): Application of mean, mode, median; coefficient of correlation, standard deviation; least squares fitting methods (both linear and non-linear regression analyses). Usage of software packages for data analysis including MS Excel, CHEMDRAW, ORIGIN, etc. Use of computational chemistry software (Gaussian 09, GAMESS); construction of z-matrix and concept of force field. Classical Molecular Dynamics (MD) simulation.

Scientific Report Writing and Publication Process (10 Hrs.): Forms and types of scientific reports. Steps involved in scientific article writing. Publication process, selection of journals. Writing research proposals and steps involved. Dissertation/Thesis writing: format, content and chapterization. Bibliography and references, referencing styles. Appendices.

Assignment: Literature survey / review writing on selected topics.

Suggested Readings

1. Kothari, C. K.; Garg, G. *Research Methodology-Methods and Techniques*, 3rd Ed., New Age International, New Delhi, 2014.
2. Kumar, R. *Research Methodology—A Step-By-Step Guide for Beginners*; 2nd Ed., Pearson Education: New Delhi, 2005.
3. Montgomery, D. C. *Design & Analysis of Experiments*; 8th Ed., Wiley India: Noida, 2013.

CHE C 602
Research and Publication Ethics

Total Credit Hours: 30
Credit: 2 (L 1 – T 0 – P 1)
Terminal Examination Duration: 2 Hours
Maximum Marks: **50** (Terminal – 25, Practical – 25)

Course objectives:

1. To help students understand the philosophy of science and ethics, research integrity, publication ethics.
2. To impart hands-on-sessions to identify research misconduct and predatory publications.
3. To acquaint the students with Indexing and citation databases, open access publications, research metrics (citations, h-index, Impact Factor, etc.) and plagiarism tools.

Learning Outcomes:

On completion of this course the students will be able to:

1. Understand the philosophy of ethics in science and scientific research, intellectual honesty and research integrity.
2. Learn to avoid scientific misconducts such as falsification, fabrication, and plagiarism.
3. Follow ethical practices in scientific publications, misrepresentation of data etc.
4. Use Indexing and citation databases, understand the importance of research metrics.
5. Handle the plagiarism software for their research work.

Philosophy and Ethics (3 Hrs.): Introduction to philosophy: definition, nature and scope, concept, branches. Ethics: definition, moral philosophy, nature of moral judgements and reactions.

Scientific Conduct (5 Hrs.): Ethics with respect to science and research. Intellectual honesty and research integrity. Scientific misconducts: Falsification, Fabrication, and Plagiarism (FFP). Redundant publications: duplicate and overlapping publications, salami slicing. Selective reporting and misrepresentation of data.

Publication Ethics (7 Hrs.): Publication ethics: definition, introduction and importance. Best practices / standards setting initiative and guidelines: COPE, WAME, etc. Conflicts of interest. Publication misconduct: definition, concept, problems that lead to unethical behaviour and vice versa, types. Violation of publication ethics, authorship and contributorship. Identification of publication misconduct, complains and appeals. Predatory publishers and journals.

PRACTICE

Open Access Publishing (4 Hrs.): Open access publications and initiatives. SHERPA/RoMEO online resource to check publisher copyright & self-archiving policies. Software tools to identify predatory publications developed by SPPU. Journal finder / journal suggestion tools viz. JANE, Elsevier Journal Finder, Springer Journal Suggester, etc.

Publication Misconduct (4 Hrs.): *Group Discussions* (2 Hrs.): Subject specific ethical issues, FFP, authorship. Conflicts of interest. Complaints and appeals: examples and fraud from India and abroad.

Software tools (2 Hrs.): Use of plagiarism software like Turnitin, Urkund and other open-source software tools.

Databases and Research Metrics (7 Hrs.): *Databases* (4 Hrs.): Indexing databases. Citation databases: Web of Science, Scopus, etc.

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.

Suggested Readings

1. Bird, A. *Philosophy of Science*; Routledge: London, U.K., 1998.
2. MacIntyre, A., *A Short History of Ethics: A History of Moral Philosophy from the Homeric Age to the 20th Century*; 2nd Ed., Routledge: London, U.K., 1998.
3. National Academy of Sciences, National Academy of Engineering and Institute of Medicine. *On Being a Scientist: A Guide to Responsible Conduct in Research*; 3rd Ed., The National Academic Press: Washington DC, USA, 2009.
4. Muralidhar, K.; Ghosh. A.; Singhvi, A. K., Eds. *Ethics in Science Education, Research and Governance*; Indian National Science Academy: New Delhi, India, 2019.

CHE OE 611
Spectroscopic Tools for Small Molecule Characterization

Total Credit Hours: 20
Credit: 2 (L 2 – T 0 – P 0)
Terminal Examination Duration: 2 Hours
Maximum Marks: **50** (Terminal – 40, Internal Assessment – 10)

Course objectives:

1. To help students understand and apply the knowledge of IR, NMR spectroscopy and mass spectrometry to elucidate the structure of an unknown compounds.

Learning Outcomes:

On completion of this course the students will be able to:

1. Prepare samples for IR & NMR spectroscopy and mass spectrometry.
2. Identify the NMR solvent residual peak and peaks arising from common organic solvents present as trace impurities in the NMR sample.
3. Elucidate the structure of an unknown organic compound from IR, NMR and HRMS data.

Spectroscopic Techniques (10 Hrs.): Revisiting the basics of IR, NMR (^1H & ^{13}C) spectroscopy and mass spectrometry, sample preparation procedures, solvent residual peak in NMR spectra, peaks of common laboratory solvents present as trace impurities in NMR samples, peak pattern and second order ^1H NMR spectra, effect of isotopes on abundance ratio of molecular ion peak in mass spectrometry.

Structural Elucidation of Small Molecules (10 Hrs.): Usage of software packages (MestReNova, Spin Works, etc.) for extraction and analysis of NMR and MS data. Structural elucidation of organic compounds from IR, NMR (^1H & ^{13}C) and HRMS (high resolution mass spectrometry) data, degree of unsaturation: index of hydrogen deficiency (IHD) and its role in structural identification.

Suggested Readings

1. Lampman, G. M.; Pavia, D. L.; Kriz, G. S.; Vyvyan, J.R., *Introduction to Spectroscopy*, 5th Ed., Cengage Learning India: New Delhi, 2015.
2. Silverstein, R. M.; Webster, F. X.; Kiemle, D. J.; Bryce, D. L., *Spectrometric Identification of Organic Compounds*, 8th Ed., Wiley India: New Delhi, 2015.

CHE OE 612 Techniques for Material Characterization

Total Credit Hours: 20
Credit: 2 (L 2 – T 0 – P 0)
Terminal Examination Duration: 2 Hours
Maximum Marks: **50** (Terminal – 40, Internal Assessment – 10)

Course objectives:

1. To make the students familiar with the principle, instrumentations and application of various characterization tools
2. To impart the knowledge of these characterization tools in the determination of physico-chemical properties of the materials
3. To help students develop their analytical skills and knowledge of characterisation techniques to evaluate the structure property relationship.

Learning Outcomes:

On completion of this course the students will be able to:

1. Understand the basic principle of the techniques and their various components and design.
2. Analyze the data and correlate it to the physico-chemical properties of the materials.
3. Identify the type of techniques required to evaluate the structure property relationship

Basic theory, instrumentation and analytical applications of the following techniques:

X-ray Diffraction Method (5 Hrs.): Powder X-Ray Diffraction (PXRD), structure determination from PXRD, phase identification, and crystallite size determination.

Electron Microscopy (4 Hrs.): Principles and application of scanning electron microscopy (SEM), transmission electron microscopy (TEM), energy dispersive analysis of X-rays (EDAX).

Surface Characterization Techniques (7 Hrs.): X-ray photoelectron spectroscopy (XPS), Auger electron spectroscopy (AES), ESCA and their applications. Brunauer-Emmett-Teller (BET) surface area analysis and adsorption isotherms, temperature programmed desorption (TPD), temperature programmed oxidation (TPO) and temperature programmed reduction (TPR), zeta-potential measurements.

Electrical properties (4 Hrs.): Polarography; cyclic voltammetry; chrono-methods; AC impedance techniques - concepts and applications.

Suggested Readings

1. Skoog, D. A.; Holler, F. J.; Nieman, T. A. *Principles of Instrumental Analysis*; 5th Ed., Cengage Learning: New Delhi, 1998.
2. Christian, G. D. *Analytical Chemistry*; 6th Ed., John Wiley and Sons: New Delhi, 2003.
3. Bard, A. J. & Faulkner, L. R.; *Electrochemical Methods: Fundamentals and Application*; 2nd Ed., Wiley India: Noida, 2006.

CHE DE 621
Chemistry of Natural Products

Total Credit Hours: 40
Credit: 4 (L 3 – T 1 – P 0)
Terminal Examination Duration: 3 Hours
Maximum Marks: **100** (Terminal – 80, Internal Assessment – 20)

Course objectives:

1. This course will deal with the classical and advanced concepts and theories of isolation and structure elucidation of biologically important pure molecules from natural products. It will be based on leading text books of the domain as well as references to current literature.

Learning Outcomes:

On completion of this course the students will be able to:

1. Extract, prepare samples for IR, UV, ^1H , ^{13}C , 2D-NMR and mass spectral studies on the natural products.
2. Elucidate the structure of an unknown medicinal products using the spectroscopic data.
3. Design synthetic strategies for synthesis of new molecules.

Introduction (4 Hrs.): Sources (plant, animal, microbial, marine) and classes of natural products.

Extraction Procedures (6 Hrs.): Conventional and modern extraction methods including maceration, percolation, Soxhlet extraction, batch extraction, continuous extraction, counter current extraction, accelerated solvent extraction and super critical fluid extraction. Concepts of extraction with respect to activity guided fractionation.

Analytical Techniques (10 Hrs.): Introduction to high performance thin layer chromatography (HPTLC), high performance liquid chromatography (HPLC), gas chromatography (GC), chiral chromatography and reverse phase chromatography. Application of these techniques in identification of markers/biomarkers.

Structure Elucidation and Synthesis (20 Hrs.): Structure elucidation of well-known bioactive molecules of natural origin by IR, UV, ^1H , ^{13}C , 2D-NMR and mass spectra and their synthesis.

Suggested Readings

1. Silverstein, R. M.; Webster, F. X.; Kiemle, D. J.; Bryce, D. L., *Spectrometric Identification of Organic Compounds*, 8th Ed., Wiley India: New Delhi, 2015.
2. Patrick, G. L., *An Introduction to Medicinal Chemistry*. 5th Ed.; Oxford University Press, New Delhi (2013).
3. Nicolaou, K. C.; Sorensen, E. J. *Classics in Total Synthesis: Targets, Strategies, Methods*; Wiley-VCH: New York, 1996.
4. Mann, J.; Davidson, R. S.; Hobbs, J. B.; Banthrope, D. V.; Harborne, J. B. *Natural Products, Their Chemistry and Biological Significance*; Longman: Essex, 1994.
5. Lemke, T. L.; Zito, S. W.; Roche, V. F.; Williams, D. A. *Essentials of Foye's Principles of Medicinal Chemistry*; Wolters Kluwer India: New Delhi, 2016.

CHE DE 622
Chemistry of Nanomaterials

Total Credit Hours: 40
Credit: 4 (L 3 – T 1 – P 0)
Terminal Examination Duration: 3 Hours
Maximum Marks: **100** (Terminal – 80, Internal Assessment – 20)

Course objectives:

1. To introduce students to the interdisciplinary field of nanoscience, properties of nanomaterials, different chemical synthetic strategies, characterization of materials and their applications.

Learning Outcomes:

On completion of this course the students will be able to:

1. Describe the different types of nanomaterials, their properties, characterization and applications.
2. Understand how surface functionalities can help nanomaterials finding appropriate technological applications.

Brief Overview of Nanomaterials (5 Hrs.): History of Nanoscience, Classification of Nanomaterials. Major challenges in nanoscience and technology.

Preparation of Nanomaterials (12 Hrs.): Preparation of nanomaterials by the following techniques:

- a) Vapour deposition
- b) Precipitation and co-precipitation methods
- c) Sol-gel methods
- d) Hydrothermal and solvothermal methods
- e) Template based synthesis
- f) Green synthetic methods

Properties of Nanomaterials (13 Hrs.):

- a) Physiochemical properties
- b) Optical properties of nanomaterials
- c) Electrical and electronic properties
- d) Magnetic properties

Application of Nanomaterials (10 Hrs.): Assembly of nanostructures and their importance for various applications. Stabilization of nanomaterials and their importance. Surface modification of nanomaterials with specific example to metal oxide nanoparticles and their significance.

Suggested Readings

1. Poole Jr., C. P.; Owens, F. J. *Introduction to Nanoscience and Nanotechnology*; Wiley India: Noida, 2020.
2. Hornyak, G. L.; Tibbals, H. F.; Dutta, J.; Moore, J. J., *Introduction to Nanoscience and Nanotechnology*; CRC Press, 2009.
3. Pradeep, T. *Nano: The Essentials: Understanding Nanoscience and Nanotechnology*; McGraw Hill Education: New Delhi, 2017.

CHE DE 623
X-Ray Crystallography for Chemists

Total Credit Hours: 40
Credit: 4 (L 3 – T 1 – P 0)
Terminal Examination Duration: 3 Hours
Maximum Marks: **100** (Terminal – 80, Internal Assessment – 20)

Course objectives:

1. To introduce students to the single-crystal X-ray crystallographic techniques and its applications.

Learning Outcomes:

On completion of this course the students will be able to:

1. Understand the basics of single-crystal X-ray structure determination techniques.
2. Solve crystal structure data, interpret and present the structural diagrams.

Crystals, Symmetry, and Space Groups (5 Hrs): The general features of crystals, symmetries of crystals, crystal systems, Bravais lattices, crystal classes, space groups, determination of space groups, cell transformations, systematic absences and information obtained therefrom.

The Basics of X-ray Diffraction (5 Hrs): Diffraction of X-rays from one-, two- and three-dimensional arrays of atoms, the reciprocal lattice, diffraction from a crystal, atomic scattering factor, structure factor.

Experimental Aspects (15 Hrs): Techniques for growing single crystals, choosing and mounting of single crystals. Intensity data collection and reduction. Structure solution: Patterson methods, direct methods. Structure refinement: least square method, R-values. Location and treatment of Hydrogen atoms, residual electron density. Disorders and twinning.

Determination and Presentation of Crystal Structure (15 Hrs.): Use of X-ray crystallographic software packages (SHELXTL, WINGX, OLEX etc.) for crystal structure determination. Presentation of structural diagrams using crystallographic software Mercury, ORTEP, PLUTON, Diamond etc. Crystallographic databases (ICSD, CSD, PDB etc.). Deposition of structural data in databases. Crystallographic Information File (CIF) and IUCR structure validation.

Suggested Readings

1. Massa, W. *Crystal Structure Determination*; 2nd Ed., Springer-Verlag: Berlin, 2004.
2. Blake, A. J.; Clegg, W.; Cole, J. M.; Evans, J. S. O.; Main, P.; Parsons, S.; Watkins, D. J. *Crystal Structure Analysis: Principle and Practice*; 2nd Ed., Clegg, W. (Ed.), Oxford University Press: New York, 2009.
3. Muller, P.; Herbst-Irmer, R.; Spek, A. L.; Schneider, T. R.; Sawaya, M. R. *Crystal Structure Refinement: A Crystallographer's Guide to SHELXL*; Muller, P. (Ed.), Oxford University Press: New York, 2006.