# Postgraduate Booklet

Department of Chemistry

Bangladesh University of Engineering and Technology (BUET)

Dhaka-1000, Bangladesh

# Contents

## Welcome Note of Head

Welcome to the **Department of Chemistry**, BUET!

Our department was founded in 1962 since the establishment of BUET as East Pakistan University of Engineering and Technology and started offering undergraduate chemistry courses for engineering students. To fulfill the national and global demands, the department introduced MPhil and PhD programs in the session of 1981-1982, followed by MSc program in 2014.

Our vibrant and evolving graduate programs provide opportunities to students in a wide area of chemical disciplines including organic, inorganic, physical, materials, environmental and at the interface of basic and applied science research. We are blessed with highly qualified, talented and inspiring faculty who are recipients of various national and international research grants. Their research efforts have been reflected in excellent publications in high-impact factor journals. In addition to research, our faculty endeavor to introduce innovative teaching methods to provide the best service in the classroom.

Apart from the academic studies and research, our graduate students get opportunities for professional development by engaging themselves in different activities such as teaching assistants in chemistry undergraduate laboratories, networking, participating in conferences and workshops, attending departmental seminars and other extracurricular activities. All these training and research experiences make our students highly competitive both for the job market and admission for higher studies in renowned universities worldwide. I wish that a student will find this department an exciting, welcoming and worthwhile place.

Dr. Md. Shakhawat Hossain Firoz
Professor and Head

# List of Faculty Members

| | Name and Designation | Research Interests |
|---|---|---|
|  | Dr. Md. Shakhawat Hossain Firoz<br>Professor & Head<br><br>shfiroz@chem.buet.ac.bd | Synthesis and Characterization of Nano-Material and Nano-Composites, Cellulose based functional materials |
|  | Dr. Md. Abdur Rashid<br>Professor<br><br>arashid@chem.buet.ac.bd | Synthetic Organic Chemistry and Synthesis of Organo-phosphorus compounds |
|  | Dr. Al-Nakib Chowdhury<br>Professor<br><br>nakib@chem.buet.ac.bd | Nano and Bio-Material, Environmental and Electrochemical aspects of Chemistry |
|  | Dr. Shakila Rahman<br>Professor<br><br>shaki@chem.buet.ac.bd | Natural Product Chemistry; Detection, Isolation and Structural Elucidation of Bio-Active Compounds |
|  | Dr. Md. Nazrul Islam<br>Professor<br><br>islammdn@chem.buet.ac.bd | Surface Chemistry, Monolayer and Micelle formation of Surfactant system |
|  | Dina Nasrin<br>Associate Professor<br><br>dina@chem.buet.ac.bd | Synthetic Organic Chemistry |
|  | Dr. Ayesha Sharmin<br>Associate Professor<br><br>ayeshasharmin900@gmail.com | Transition metal based luminescent novel Probes, drug delivery system, electrochemistry, chemical biology |

| Name and Designation | Research Interests |
|---|---|
|  Dr. Chanchal Kumar Roy<br>Assistant Professor<br>ckroy@chem.buet.ac.bd | Hydrogels, Electrochemistry, Supramolecular Chemistry, Polymer Chemistry, Adhesives, Supramolecular Chemistry, Supercapacitor, Battery |
|  Dr. Sharmeen Nishat<br>Assistant Professor<br>snnupur@chem.buet.ac.bd | Organic Chemistry, Carbohydrate Chemistry, Environmental Chemistry, Chemical Biology, Immunology, Microbiology, Hydrogel |
|  Dr. Md. Abdul Goni<br>Assistant Professor<br>abdulgonichem@gmail.com | Analytical and Environmental Chemistry, Organometallic Chemistry, Homogeneous and Heterogeneous Catalysis, Material Chemistry |
|  Dr. Md. Ayub Ali<br>Assistant Professor<br>shuvro070@chem.buet.ac.bd | Catalysis, Organic Synthesis, Material Chemistry, Organometallics, Transition metal. |
|  Md. Kausar Ahmed<br>Assistant Professor<br>kausar55@chem.buet.ac.bd | Material Chemistry (synthesize and characterization of polymers) |
|  Dr. Md. Mahbub Alam<br>Assistant Professor<br>mdmahbub@chem.buet.ac.bd | Polymer Chemistry |

**Faculty on leave**

| | |
|---|---|
| Dr. Abu Bin Imran | Associate Professor |
| Dr. Md. Shafiul Azam | Assistant Professor |
| Dr. Md. Elius Hossain | Assistant Professor |
| Md. Abu Hasan Howlader | Assistant Professor |
| Nahida Akter | Assistant Professor |

**List of Staffs**

| | |
|---|---|
| Mr. Md. Mamun-or Rashid | Senior Technical Officer |
| Mr. Md. Kabir Hossain | Lab. Instructor Cum-Store-keeper |
| Mr. Md. Abdur Razzaque | Store Keeper |
| Mr. Md. Masud Hasan | LDA Cum-Computer Operator |
| Mr. Md. Showkat Ali | Senior Lab. Attendant |
| Mr. Md. Shamsul Haque | Senior Lab. Attendant |
| Mr. Md. Alamgir Hossain | Senior Lab. Attendant |
| Mr. Nuruddin Bhuiyan | Senior Lab. Attendant |
| Mr. Md. Moniruzzaman Sarkar | Lab. Attendant |
| Mr. Md. Tarikuzzaman | Lab Attendant |
| Mr. Golam Rasul | MLSS |
| Mr. Md. Mosharof Hossain | Office Attendant |

## Introduction of Postgraduate Programs

The Department of Chemistry, BUET offers three post-graduate degree programs in Chemistry including Doctor of Philosophy (Ph.D.), Master of Philosophy (M.Phil.) and Master of Science (M.Sc.). Students from various selected disciplines are eligible for admission into these programs as full time or part time students following fulfillment of minimum requirements. Students, serving in different organizations are allowed to be admitted as part time students with the written consent of the employer. The final selection of candidates for admission into the graduate programs will be based on either oral or written exam depending on the condition set by selection committee as constituted by the Board of Post Graduate Studies (BPGS). After selection, supervisor or advisor will be assigned to the students who will provide guidance to the respective students in all academic affairs. Students are required to pay academic fees according to university rules and regulations, afterward complete courses registration by consulting with assigned advisor/ supervisor within two weeks from the commencement of a semester. Full time students must register for a minimum of 12 credit hours and a maximum of 15 credit hours per semester. Part time students must register for a minimum of 6 credit hours and a maximum of 9 credit hours per semester. Course evaluation strategy would be determined by the relevant course teacher, which may include class test, quiz, viva, presentation along with a written exam. Course evaluation will be reflected as GPA.

## Doctor of Philosophy (Ph.D.) Degree in Chemistry

***Registration***

Selected candidates should get registered with the University and pay the fees as per the University rules before the commencement of each semester enrollment. Course registration must be completed within two weeks from the start of the semester.

***Appointment of a Supervisor***

On provisional admission, Selection Committee will submit a name of a supervisor who will be a full-time member of the staff belonging to the department. The supervisor will prescribe a plan of study to be undertaken by the student and supervise the progress of the candidate's work.

***Academic Requirements and Regulations***

The minimum duration of the Ph.D. course will be four semesters from the date of provisional admission. A student must complete all requirements for the Ph.D. degree within six academic years (session) from the date of his provisional admission. Academic progress will be measured in terms of credit hours earned by the student. One Credit hour subject will require 14 hours of lecture for one semester while one Credit hour for thesis work would require 42 hours of research work for one semester. The number of credit hours for each subject has been

specified in the syllabus of the department. A student must complete a minimum of 54 credit hours of which 45 credit hours will be assigned for a thesis. Candidates having one-year M.Sc. degree must complete another 12 credit hours as non-credit. There will be two categories of students, namely, full-time students and part-time students. A candidate serving in different organizations can be enrolled as a part-time student with the written consent of the employer. A part time student will be assigned a maximum of 9 credit hours of course including thesis work in any semester. Full-time students will have to register for a minimum of 12 credit hours and a maximum of 15 credit hours per semester. A full-time student will not be allowed to be in the employment of any organization (even as a part-time employee). However, they may be employed as Teaching/Research Assistant at the University. If a full-time student becomes an employee (full time or part time) of any other organization in the middle of a semester, he/she may, with the approval of the Head/Director of the Department/Institute and his/her Employer, be allowed to continue as a full-time student for that semester. A student may be allowed to switch from part-time to full-time or vice versa on the recommendation of the respective Doctoral Committee before the commencement of a semester.

***Doctoral Committee***

A Doctoral Committee for every student will be proposed by the Supervisor in consultation with the Head of the department. The Doctoral Committee should meet from time to time at the request of the Supervisor to review the progress of the student.

***Research Proposal***

The student, after passing the comprehensive examination, has to submit a research proposal to the Doctoral Committee. The Doctoral Committee will examine the proposal and recommend changes if necessary.

***Examination***

In addition to tests, assignments and/or examinations during the semester there will be a written examination for each of the subjects in a semester at the end of that semester. The final grade in a subject will be based on the performance in all tests, assignments and/or examinations.

***Qualifying Requirements***

***Course Work***

To qualify for the degree a student must earn a minimum grade point average (GPA) of 2.75 based on the weighted average of grade points (GP) in his / her course work. A student will not be allowed to continue the programme if he/she obtains a total of three or more F grades in one or more than one subject taken together, during the course of his / her studies.

***Comprehensive Examination***

Comprehensive examination will be held after the completion of the course work by the student. The comprehensive examination will be comprised of a written examination and/or an oral examination to test the knowledge of the student in his/her field of study and research.

***Thesis***

At the end of the student's research work, the student shall submit a thesis that must be an original contribution to engineering/sciences and worthy of publication. On completion of the research work and submission of the thesis, an oral examination shall be arranged.

***Program outcome (PO) of Doctor of Philosophy in Chemistry***

- An ability to understand fundamentals and applications of current chemical theories for the physical world.
- An ability to perform a literature search, extract useful information to develop research methodology.
- An ability to design and execute new chemical experiments with high degree of sophistication, good laboratory practice and proper handling of chemicals to successfully complete an advanced research project.
- An ability to identify and analyze the scientific problems and successfully carry out experiments, as well as to analyze and interpret data to arrive at scientific results.
- An ability to author manuscripts describing their research and its impacts that are suitable for publication in peer reviewed scientific journals, and to communicate and share knowledge of chemistry at global chemistry community.
- An ability to integrate their knowledge from each of these areas with critical thinking skills in order to become problem solvers.
- An ability broadens their professional foundations through activities such as teaching, internships, fellowships, mentoring and research grant applications.
- An ability to acquire the tools to become fully independent chemical researchers.
- An ability to work effectively in teams and provide leadership
- An ability to solve any national problems in chemical issues.
- An understanding of professional responsibility and ethics in Chemistry.

## Master of Philosophy (M. Phil.) in Chemistry

***Registration***

Selected candidates should get registered with the University and pay the fees as per the University rules before the commencement of each semester enrollment. Course registration must be completed within two weeks from the start of the semester.

***Appointment of Advisor/Supervisor***

After admission, each student will be assigned, by the BPGS committee, an Adviser from among the teachers of the Department not below the rank of an Assistant Professor who will

be a full-time member of the staff belonging to the department. The Advisor will prescribe a plan of study to be undertaken by the student. To complete the thesis, work a student must choose a supervisor from the department. Supervise will monitor and supervise the research work. Students are suggested to communicate with their prospective supervisor within the first semester.

***Academic Requirements and Regulations***

The minimum duration of the M. Phil course will be four semesters. A candidate for the M. Phil degree must complete all the requirements for the degree within five academic years (Session) from the date of the first admission in the respective program. Academic progress will be measured in terms of credit hours earned by a student. One credit hour course will require 14 hours of lecture for one semester; while one credit hour for thesis/ laboratory would require 42 hours of work for one semester. The number of credit hours for each course will be as specified in the syllabus of the department. A student must earn a minimum of 48 credit hours including a thesis for which 30 credit hours will be assigned. There will be two categories of students, namely, full-time students and part-time students. A candidate serving in different organizations can be enrolled as a part-time student with the written consent of the employer. A part time student will be assigned a maximum of 9 credit hours of course including thesis work in any semester. Full time students will have to register for a minimum of 12 credit hours and a maximum of 15 credit hours per semester. A full-time student will not be allowed to be in the employment of any organization (even as a part-time employee). However, they may be employed as Teaching/Research Assistant at the University. If a full-time student becomes an employee (full time or part time) of any other organization in the middle of a semester, he/she may, with the approval of the Head/Director of the Department/Institute and his/her Employer, be allowed to continue as a full-time student for that semester. A student may be allowed to switch from part-time to full-time or vice versa on the recommendation of the respective BPGS Committee before the commencement of a semester.

***Conduct of Examination***

In addition to tests, assignments and/or examinations during the semester will be given by the teacher(s) concerned which will be a written examination and/or other tests for each of the courses offered in a semester. The final grade in a subject will be based on the performance in all tests, assignments and / or examinations.

***Qualifying Requirements***

***Course Work***

The qualifying requirement for graduation is that a student must earn a minimum grade point of 2.65 based on the weighted average in his course work. A student will not be allowed to continue the programme if he/she obtains a total of three or more F grades in one or more than one subjects taken together, during the course of his / her studies. In addition to

successful completion of course works every student must submit a thesis on his/her research work fulfilling the requirements as detailed in the following sections.

***Thesis***

Research work for a thesis will be carried out under the supervision of a full-time faculty member belonging to the department. The thesis proposal of a student has to be submitted for approval of the CASR, after completion of at least 12 credit hours of course work. The research work must be carried out in this University or at a place(s) recommended by the BPGS. The thesis should demonstrate an evidence of satisfactory knowledge in the field of research undertaken by the student. Every student submitting a thesis in partial fulfillment of the requirements of a degree shall be required to appear at an oral examination in form of a presentation in front of an examination board decided by CASR, on a date or dates fixed by the Supervisor. In addition to the above procedure, every student have to present their research plan immediately after the completion of the first semester and research work before the oral examination as decided by the BPGS.

***Program Outcome (PO) of Master of Philosophy in Chemistry***

- An ability to understand the advanced theories, concepts and applications of chemistry.
- An ability to apply knowledge of important laboratory techniques, methods, and instrumentation.
- An ability to perform a literature search, extract useful information to develop research methodology.
- An ability to design and execute new chemical experiments with high degree of sophistication, good laboratory practice and proper handling of chemicals to successfully complete an advanced research project.
- An ability to identify and analyze the scientific problems and successfully carry out experiments, as well as to analyze and interpret data to arrive at scientific results.
- An ability to communicate and share knowledge of chemistry both orally and in writing.
- An ability to write research articles.
- An ability to integrate their knowledge from each of these areas with critical thinking skills in order to become problem solvers.
- An ability to broaden their professional foundations through activities such as teaching, internships, and fellowships.
- An ability to work effectively in teams and provide leadership.
- An ability to contribute any national problems in chemical issues.
- An understanding of professional responsibility and ethics in Chemistry.

# Master of Science (M.Sc.) in Chemistry

***Registration***

Selected candidate should get registered with the University and pay the fees as per the University rules before the commencement of each semester enrollment. Course registration must be completed within two weeks from the start of the semester.

***Appointment of Advisor/Supervisor***

After admission, each student will be assigned, by the BPGS committee, an Adviser from among the teachers of the Department not below the rank of an Assistant Professor who will be a full-time member of the staff belonging to the department. The Advisor will prescribe a plan of study to be undertaken by the student. To complete the thesis, work a student must choose a supervisor from the department. Supervise will monitor and supervise the research work. Students are suggested to communicate with their prospective supervisor in the first semester.

***Academic Requirements and Regulations***

The minimum duration of the M.Sc. program will be three semesters. A candidate for the M.Sc. degree must complete all the requirements for the degree within five academic years (Session) from the date of the first admission. Academic progress will be measured in terms of credit hours earned by a student. One credit hour subject will normally require 14 hours of lecture for one semester; while one credit hour for thesis/project/ laboratory would normally require 42 hours of work for one semester. An M. Sc. student is required to complete 6 courses of 18 credits in Chemistry. Besides these courses, a student has to submit a dissertation equivalent to 18 credits on his/her research findings.

***Conduct of Examination***

In addition to tests, assignments and/ or examinations during the semester, there will be a written examination and / or other tests for each of the subjects offered in a semester at the end of that semester. The final grade in a subject will be based on the performance in all tests, assignments and / or examinations.

***Qualifying Requirements***

***Course Work***

The qualifying requirement for graduation is that a student must earn a minimum grade point of 2.65 based on the weighted average in his course work. A student will not be allowed to continue the programme if he/she obtains a total of three or more F grades in one or more than one subject taken together, during the course of his / her studies. In addition to successful completion of course works every student has to submit a thesis on his research work, fulfilling the requirements as detailed in the following sections.

***Thesis***

Research work for a thesis has to be carried out under the supervision of a full-time member of the staff belonging to the department. The thesis proposal of a student has to be approved by CASR, after completion of at least 12 credit hours of course works. The research work must be carried out in this University or at a place(s) recommended by the BPGS / RAC. The thesis should demonstrate evidence of satisfactory knowledge in the field of research undertaken by the student. Every student submitting a thesis in partial fulfillment of the requirements of a degree shall be required to appear at an oral examination on a date or dates fixed by the Supervisor concerned. In addition to the above procedure, all students have to present their research plan immediately after the completion of the first semester and research work before the oral examination as decided by the BPGS.

***Program Outcome (PO) of Master of Science in Chemistry***

- An ability to understand the fundamental theories, concepts and applications of chemistry.
- An ability to apply knowledge of important laboratory techniques, methods, and instrumentation.
- An ability to perform a literature search, extract useful information to develop research methodology.
- An ability to design and execute new chemical experiments, good laboratory practice and proper handling of chemicals to successfully complete a research project.
- An ability to identify and analyze the scientific problems and successfully carry out experiments, as well as to analyze and interpret data to arrive at scientific results.
- An ability to communicate and share knowledge of chemistry both orally and in writing.
- An ability to broaden their foundations through activities such as teaching, internships, and fellowships.
- An ability to work effectively in teams and provide leadership.
- An ability to contribute any national problems in chemical issues.
- An understanding of professional responsibility and ethics in Chemistry.

## Grading system for postgraduate studies

Final grades for courses shall be recorded as follows:

| Grade | Merit description | Grade points |
|---|---|---|
| A(Plus) | Excellent | 4.0 |
| A | Very good | 3.5 |
| B(Plus) | Good | 3.0 |
| B | Average | 2.5 |
| C | Pass | 2.0 |
| F | Failure | 0.0 |

| | | |
|---|---|---|
| I | Incomplete | - |
| S | Satisfactory | - |
| U | Unsatisfactory | - |
| W | Withdrawn | - |

Courses in which the student gets F grades shall not be counted towards credit hour requirements and for the calculation of Grade Point Average (GPA). Performance in all the subjects including all the F grades shall be reflected in the transcript.

## Instrument Facilities

| | |
|---|---|
| UV-Visible Spectrophotometer | Thermostat Bath |
| FTIR | Freeze Dryer |
| Potentiostat/Galvanostat | Vacuum Oven |
| Polarimeter | Ultrasonic Bath |
| Universal Testing Machine | Drying Oven |
| Fiber Optic Spectrometer | Ostwald Viscometer |
| High speed centrifuge | Oven |
| Density Meter | Mechanical Stirrer |
| High temperature furnace | Shaker |
| Incubator | Orbital Shaker |
| Immersion Bath Circulator | Combined Meter |
| Tensiometer | Conductivity Meter |
| Electrochemical Analyzer | Kjeldahl Apparatus |
| Balance | Rotary Evaporator |
| PH meter | Hot Plate with Magnet |

I addition to the above facilities students has access to different paid service of FESEM, XRD, NMR, DSC, TGA etc in BUET, University of Dhaka, BCSIR and Atomic Energy Commission. CASR, BUET will provide financial support.

## Financial Assistance for Students

Financial assistance is available for the poor and meritorious students. Students can apply for different scholarships from the University. Research Assistantships and Teaching Assistantships are available in the Department, which are selected on the basis of academic results. Research Assistantship is also available in different laboratories run by the faculty members. BUET has its own M.Sc., Ph.D. and Foreign Fellowships for local and foreign students. In addition to that, students can apply for different Government Fellowship programs recommended by their supervisors.

## Accommodation

Limited number of seats is available for allotment of post-graduate students in BUET. After getting admission students has to apply to Hall Provost for allotment. Shahid Smriti Hall is assigned for male students and Chatri Hall is assigned for female students. Besides the university accommodation, students can seek private accommodation near the university area.

## Alumni Association

The Department of Chemistry, BUET has established an Alumni Association to create strong bonds and social interaction with its well-wishers. The students who graduated from this department are eligible for being a member of this association. Students are advised to get registered to the association after their graduation. To foster the interaction of students with their alumni, different kinds of programs are organized from time to time. Check the following link for details: chem.buet.ac.bd/alumni

## Syllabus

### Organic Branch

**Chem 6001** **Chemistry of Natural Products**

3.00 Credits, 3 hours/week

Terpenes: Chemistry of important terpenes from various groups, e.g., Humulene, Germacrone etc. Alkaloids: Structure and synthesis of some important alkaloids. Steroids: Synthesis, spectral properties, configuration and reactions of steroids, hormones, growth regulators, biosynthesis of sterols.

**Chem 6002** **Chemistry of Biomolecules**

3.00 Credits, 3 hours/week

Amino acids, structure and bio-synthesis of proteins, purines, nucleic acids and nucleoproteins. Fundamental role of nucleic acids in life processes, structures of DNA and RNA and their function, lipids and phospholipids.

**Chem 6003** **Organic Reagents in Synthesis**

3.00 Credits, 3 hours/week

Use of some of the more important organic and inorganic reagents in organic synthesis. Exercises in the synthesis of C-C, C-O, C-X, C-N, C-S and C-P bonds. Exercises in the synthesis of complex molecules of nature.

**Chem 6004** **Carbohydrate Chemistry**

3.00 Credits, 3 hours/week

Configuration assignments and conformational analysis of mono and disaccharides. Use of optical methods including Hudson's rule of isorotations and Lactone rule. Reactions of sugars including their actions with acids and bases. Esters, ethers and acetals of sugars. Anhydro-sugar, branched chain sugar, unsaturated sugar, deoxy-sugar and polyamine sugar.

Polysaccharides: Structural investigation and group analysis, Barry and Smith degradation, molecular weight determination etc. Amylose and amylopectin, cellulose, hemicullulose, glycogen and inulin. Sulphated polysaccharides and marine algal polysaccharides.

**Chem 6005 Spectroscopy and Structure of Organic Molecules**

3.00 Credits, 3 hours/week

UV Spectroscopy: Principle of measurement, electron excitation, simple chromophore groups, conjugated systems and aromatic systems. IR spectroscopy: Vibration spectra, factors affecting IR frequencies and applications. NMR spectroscopy: Introduction, nuclear overhauser effect, shift reagents, dynamic polarization and interpretation of the spectral data. Mass spectrometry: Theory, spectrometer and application to structure determination of organic molecules. Application of all the spectroscopic methods in following the progress of reactions by diagnostic appearance and disappearance of functional groups in organic compounds and also in characterizing the products. Application of spectroscopy in the elucidation of the structure of organic compounds.

**Chem 6006 Advanced Organic Reaction Mechanism**

3.00 Credits, 3 hours/week

Structure and bonds in organic molecules, localised and nonlocalised bonds in terms of molecular orbital theory. Orbital symmetry and chemical reactions, electrocyclic, cyclo-addition and sigmatropic reaction. Free radical reactions: mechanism of free radical reactions in substitution, addition, rearrangement and oxidation reactions. Photochemical reactions; isomerization and molecular rearrangement.

**Chem 6007 Advanced Stereochemistry**

3.00 Credits, 3 hours/week

(i) Symmetry elements, point groups (ii) Optical activity – its origin, atomic and conformation asymmetry (iii) Variation of optical activity with wave length. Optical rotatory dispersion and circular dichroism curves and their application in determining the configuration and conformation of different compounds (iv) Conformational analysis, reactivity of alicyclic, cyclic, fused and bridged ring systems. Curtin Hammet principle and its application in determining the course of reaction in different compounds (v) Tricovalent carbon (vi) Optical activity due to atoms other than carbon.

**Chem 6008 Kinetic and Energetics of Organic Reactions**

3.00 Credits, 3 hours/week

(i) Thermodynamic considerations and study of energetics of organic reactions, kinetics of organic reactions, consecutive reactions, the steady state approximation, parallel reactions, entropy of activation in conjunction with energy of activation particularly in reactions leading to cyclisation (ii) Variation in kinetics in acid and base catalyzed reactions, microscopic reversibility, correlation of reaction rates and equilibria (iii) Solvent effects (iv) Isotopic effects (v) Linear free energy relationship (vi) Application of the above concepts to substitution, addition and elimination reactions.

**Chem 6009** **Organo-Metallic Chemistry**

3.0 redits, 3 hours/week

Nature of carbon metal bonding systems, structures and reactions of organo-metallic compounds. Organo-metallic reagents in organic synthesis. A general introduction to the types and nature of carbon metal bonding systems. Structures and reactions of: The alkali metal organo-metallic with special reference to organo-lithium. The alkaline earth metal compounds with special reference to organo-magnesium reagents. The main group (IV) organo-metallics with special reference to organosilicon compounds. Organic compounds of transition metals: Reactions, structure, nature and stability etc. of complexes. A brief study of organo-phosphorus, antimony and bismuth compounds.

**Chem 6010** **Chemistry of Heterocyclic Compounds**

3.00 Credits, 3 hours/week

Types of hetero-atomic structures, criterion of hetero-aromaticity, concept of abundancy and deficiency. Reactivity of hetero-atoms, role of hetero-cycles and hetero-atoms as substituent and conductor of electronic effect. Chemistry of three, four and five membered hetero-cycles, condensed five membered hetero-cycles, five-membered ring hetero-cycles with more than one hetero-atom. Pyridine, quinoline and isoquinolinecompounds. Addition to the cyano group to form heterocycles, tautomerism in purines, hydroxythiophene and hydroxy furan systems. Synthesis of heterocycles involving cyclo-addition reactions, heterocycles of biological interest.

**Chem 6011** **Biogenesis and Biosynthesis of Natural Product**

3.00 Credits, 3 hours/week

Introduction to primary and secondary metabolites, precursors. Methods used in study of biosynthesis, chemical speculation, seasonal variation, organisms with blocked biosynthesis pathways, feeding experiments, measurement of the efficiency of precursors and studies with enzymes, feed back and other regulatory mechanisms.

Acetongenins-construction of acetate hypothesis, biosynthesis of saturated, unsaturated, fatty acids, polyacetylenes and aromatic polyketides. Isoprenoids-biosynthesis of mevallanat, the biological isoprene unit, alkylation of non-isoprenoids, alkylation, polymerization of isoprenoids, tail to tail linkages and cyclization of poly isoprene chains to mono, sesqui, diandtriterpenes etc. Modifying reactions of triterpenes and steroids. Shikimic metabolites (phenyl propanoids), simple cinnamic acid derivatives, flavonoids, coumarins, carotenoid, tropolones, lignins etc. Alkaloids and other amino acid derivatives, alkaloids based on aliphatic amino acids, based on aromatic amino-acids, alkaloids derived from trytophan, other amino acid derivatives and peptide derivatives. Methods precursor incorporation experiments in fungi, biosynthesis in cell free systems and biosynthesis in mutant organism.

**Chem 6012** **Spectra of Organic Compounds**

3.00 Credits, 3 hours/week

Introduction to electromagnetic spectrum, ultraviolet spectroscopy, electronic transition, simple chromophoric groups, conjugated systems, aromatic systems, use of UV spectra in structure determinations. Infra-red spectroscopy, molecular vibrations and their interaction with infrared radiation, interpretation of IR spectra. Nuclear magnetic resonance spectroscopy, magnetic properties of nuclei, the chemical shift, spin-spin interactions, nuclear magnetic double resonance, interpretation of the spectra of organic molecules. Mass spectroscopy, the production analysis of positive ions, molecular ion, application of isotopic abundance measurements, fragmentation modes of mass spectra of some representative compounds. The effect of stereochemistry on the above spectra will be discussed in each case.

**Chem 6013** **Organic Synthesis**

3.00 Credits, 3 hours/week

Formation of carbon-carbon single bond via reactions of enolate anions, enamine reactions, bisthiocarbonions 1,4-addition of organo-metallic compound of lithium diakyl- and diaryl-cuprates, carbenes and carbenoids and photocyclisation. Formation of C=C bonds via elimination, oxidative decomposition reactions. Thermal and photosensitisedDiel's Alder reaction, its mechanism and stereochemistry, the "One" synthesis. Oxidation reaction: Selective oxidation of hydration of hydrocarbons, olefines, alcohols, Baeyer Villigre, photosensitised oxidation of olefines. Reduction reactions: selective catalytic hydrogenations dissolving metal reductions, hydride-transfer reductions. Examples: stereospecific synthesis, synthesis of naturally occurring compounds.

**Chem 6014** **Stereochemistry and Reactivity of Organic Compounds**

3.00 Credits, 3 hours/week

Structure and symmetry point groups, stereoisomerism, optical isomerism, racemic modification, diastereoisomers, torsional isomerism, allotropisomers, absolute configuration, conformational analysis, conformation and reactivity, stereochemistry of ring systems, fused rings, allenes, macromolecules of tri-covalent carbon. Optical rotatory dispersion, circular dichroism and their application. stereo-specific and stereo-selective synthesis. Stereochemistry and mechanism of reactions.

**Chem 6015** **Chromatography Principle and Application**

3.00 Credits, 3 hours/week

Fundamental types of chromatography: Liquid partition chromatography, thin layer and reversed phase partition chromatography. Chemical constitution and $R_f$ value. Adsorption chromatography, gas liquid chromatography, column efficiency and resolution, various types of detectors, preparative, programmed temperature gas chromatography, exclusion chromatography, gel permeation and ion exclusion techniques, ion exchange chromatography. Exchange equilibria plate theory, applications, electrophoresis and electro-chromatography, mechanisation and automation of column chromatography. Solutions of different problems by chromatographic methods.

**Chem 6016** **Advanced Topics in Chemistry**

3.00 Credits, 3 hours/week

**Chem 6017** **Organic Pollutants**

3.00 Credits, 3 hours/week

Degradation of different components of biosphere by environmental pollutants; a general overview of interconnections among biosphere, atmosphere, antrosphere, hydrosphere and geosphere. Pollution by Hydrocarbons: chemical nature, dispersion, evaporation, photooxidation & microbial transformation to the environment. Petroleum & aquatic organisms, biphenyl & polychlorinated biphenyls (PCBs), physical and chemical properties, environmental distribution and behavior. Polycyclic aromatic hydrocarbon; chemical nature, occurrence and behavior in the environment, carcinogenicity and toxicity of PAHs, effect on human and the natural environment. Pollutants from Industries: their treatment by chemical, physical, thermal and photochemical method with special references to polymers & plastic, soap & detergents, chemical & pharmaceutical and pulp & paper industries. Waste Materials; nature, sources and environmental chemistry of hazardous wastes, hazardous wastes in atmosphere hydrosphere and biosphere, microbial metabolism in waste degradation, appropriate disposal by proper chemical & biological treatment of city waste, domestic & hospital wastes. Fertilizers: nitrogenous, phosphatic fertilizers. Environmental implications of fertilizer, abatement procedure of fertilizer pollution. Organic pollutants in vegetables, fruits and other food materials. Insecticides, fungicides, herbicides, and their effects on environment and human health with reference to DDT, Heptachlor, Endosulfan, Diazinon, Malathion, Parathion, etc. Formulation, mechanism of action and metalbolism of pesticides biological system. Toxicology; introduction to toxicology, dose-response relationship, dose & frequency of use. Maximum Recommended level (MRL) and Acceptable Daily intake. Integrated pest management (IPM): definition, key components of IPM, pest control techniques, reduction of pollution.

**Chem 6018** **Medicinal Chemistry**

3.00 Credits, 3 hours/week

Receptors and drug action: role of receptor, receptor families, neurotransmitters, design of agonists and antagonists, and receptor and the biological response. Drugs acting on DNA; antimetabolites, enzyme inhibitors, intercalating agents, alkylating agents, antisense drugs, and chain-cleaving agents. Quantitative structure activity relationship (QSAR); introduction, physiochemical properties, Hanch equation, the Craig plot, bioisosteres, and planning a QSAR study. Combinatorial synthesis for drugs: introduction, basic of combinatorial synthesis, design of combinatorial synthesis, the solid phase synthesis, and combinatorial synthesis in solution. Immunobiologicals: Cells of the immune system, immunity, acquisition of immunity. Allergy: introduction, histamines, types of allergens, antihistamic agents, and inhibition of histamine release. Cancer and cancer chemotherapy: definition, principles, biochemical basis of cancer, cancer therapy, and class of anticancer agents. Medicinal chemistry of herbs: herb, purity and standardization, herb as a drug, types of herbs, and

chemistry and pharmacological activity of some herbs. Pharmaceutical Chemistry: introduction, pharmacopoeias, types of analytical methods used for the determination of the purity of pharmaceutical substances, pharmacopoeial assay, example of some pharmacopoeial assays in relation to British Pharmacopoeia – Aspirin, Paracetamol, Ascorbic acid, Ampicillin, Metronidazole.

**Chem 6019 Food Chemistry**

3.00 Credits, 3 hours/week

General introduction to food chemistry, basic food groups. Quality and choice of food, Food safety and security. Milk and dairy products: types of milk, processing of milk. Product of fermented milk; Sour milk, yoghurt, cheese etc. Cereals and cereal products; introduction, origin, chemical composition, celiac diseases. Fruits and Fruits Product: composition, nitrogen containing compounds, carbohydrates, vitamin and mineral in fruits, chemical changes during ripening of fruits, ripening as influenced by chemical agents. Fruit products preparation and preservation; dried fruits, canned fruits, fruit juices, fruit juice beverages, lemonades. Caffeine containing beverages. Protein in foods; fish, meat, and eggs. Lipids; edible fats, oils and other lipids-their occurrence and composition in foods, their effects on health. Coffee, Tea, Cocoa; coffee and coffee substitutes, tea and tea like products, cocoa and chocolate. Spices, salt and vinegar: composition, occurrence and production. Food additives: vitamins, amino acids, minerals, aromatics substances, flavor enhancer, food colors, antioxidants, thickening agents, gel builders, stabilizers, bleaching agent. Food contamination: toxic trace elements, toxic compounds of microbial origin, pesticides, medicines and feed additives, cleansing agents and disinfectant.

## Physical-Inorganic Branch

**Chem 6101 Chemistry of Coordination Compounds**

3.00 Credits, 3 hours/week

Theories of coordination: valence bond theory, crystal field theory, ligand field theory and molecular orbital theory Detailed study of different types of complexes. Stability constant of complexes: different methods of determination of stability constant, application of stability constants in different fields, e.g., life sciences, medicine, pollution, electrochemistry, analytical chemistry, geochemistry etc.

**Chem 6102 Modern Methods of Chemical Analysis**

3.00 Credits, 3 hours/week

Application of electro-analytical methods in chemical analysis. Application ofUV-visible, IR spectrophotometry, flame photometry, atomic absorption spectroscopy, turbidimetry, nephelelemtry, optical rotatory dispersion/circular dichroism, NMR, Mass spectrometry, DTA and TGA in chemical analysis. Principles of gas chromatography and its applications.

**Chem 6103 Corrosion Science**

3.00 Credits, 3 hours/week

Thermodynamics of corrosion; kinetics of hydrogen evolution and oxygen reduction reaction; hydrogen overvoltage, electrode kinetics, pourbais diagram, theories of homogeneous corrosion and local cell reaction; corrosion in acidic, neutral and alkaline media. Role of inhibitors and alloying elements. Principles governing cathodicprotection.Mechanism of atmospheric oxidation of metals and alloys.Study of selected systems of industrial importance.

**Chem 6104 Studies on Crystal and Molecular Structure by Diffraction Methods**

3.00 Credits, 3 hours/week

Classification of crystals, crystal shapes, lattices and unit cells, crystal planes, methods used in crystal structure studies. Principles and application of electron microscopy, electron diffraction, X-ray diffraction and neutron diffraction. Advanced methods of X-ray data collection. Patterson functions, image seeking functions and their use in structure analysis:

**Chem 6105 Advanced Electrochemistry**

3.00 Credits, 3 hours/week

Activity and activity coefficient, activities of electrolytes.The Debye-Huckel theory.Extension of the Debye-Huckel treatment, weak Electrolytes and the Debye-Huckel theory. Electrolysis and Polarization: Electromotive force and cells, thermodynamic data from cell e.m.f.; polarization, deposition potential, determination of anode and cathode potentials, decomposition voltage of aqueous of solution. Processes at electrodes. Theories of overvoltage, mechanism of anodic and cathodic age. Rate of growth of overvoltage.The deposition and corrosion of metals. Physical nature of electrodeposition. Separation of metals by electrolysis. Electrochemical passivity and theories of passivity.

**Chem 6106 Chemistry of Polymer**

3.00 Credits, 3 hours/week

Polymers: polymerization reactions, kinetics of polymerization reactions, characterization, solubility chart for identification of polymer, specific chemical tests for various polymers, thermal behaviours of polymers; DTA and TGA studies, mechanical behaviour of polymers, visco-elastic studies, size and shape of macromolecules, internal frictions, swelling phenomenon and crosslink density. Molecular weight determination using viscometry. Osmometry. Light scattering, ultracentrifuge and gel permeation chromatography. Methods to study tacticity, stereoregularity and crystallinity, Electrical resistivity and dielectric behaviour.

**Chem 6107 Chemical Kinetics and Solution Thermodynamics**

3.00 Credits, 3 hours/week

(a) Order of reaction and practical measurement of reaction rate. Kinetics and mechanism of complex reactions.Effect of temperature on reaction rate. (b) Analysis of the different laws of thermodynamics and its application to chemical systems, properties of Gibbs function. Thermodynamics of solution and partial molal quantities. Thermodynamics of mixing.

**Chem 6108** **Chemistry of Pollution**

3.00 Credits, 3 hours/week

Chemical equilibrium principles applied to the chemistry of natural and polluted water and to the chemistry of water treatment. Analytical methods applied in the control of water and air pollution. Principles of chemical separations involving adsorption, ion-exchange chromatography, solvent extraction methods. Fundamental concepts of adsorption, ion-exchange chromatography, solvent extraction methods, fundamental concepts of adsorption and emission spectroscopy. Industrial toxins and their toxicology. Classification and analysis of inorganic and organic toxins. Radiation hazards, air pollution and analysis. Social and economic aspects of pollution.

**Chem 6109** **Surface Chemistry**

3.00 Credits, 3 hours/week

Surface growth, the role of defects in the growth of surface, surface composition. Techniques to determine surface composition: high vacuum techniques, electron energy loss spectroscopy, auger electron spectroscopy, low energy electron diffraction technique, scanning electron microscopy and scanning tunneling microscopy. Adsorption at solid surface: Langmuir and BET isotherms, adsorption kinetics and adsorption processes. Catalytic activity at surfaces: Eley-Ridel mechanism, Langmuir-Hinshelwood mechanism, the significance of volcano curve and catalysis in the industrial processes. Redox processes mediated by surface, conventional and new materials for electrode surface.

**Chem 6110** **Aquatic Chemistry**

3.00 Credits, 3 hours/week

Scope of aquatic chemistry in different fields, the solvent water, aspects of chemical thermodynamics, kinetics, acidity and alkalinity. Dissolution of carbon dioxide, atmosphere-water interactions. Metal ions in aqueous solution and ionic equilibrium in aqueous system, aspects of co-ordination chemistry, precipitation and dissolution, redox condition in natural water and microbial radiation. The solid-solution interface: adsorption, dissolution of minerals, nucleation and crystal growth. Trace metals: cycling, regulation and biological role and photochemical process. Particle-particle interaction: colloids, coagulation and filtration, regulation of chemical composition of natural water. Chemical context of water quality.

**Chem 6111** **Bio-inorganic Chemistry**

3.00 Credits, 3 hours/week

General principles: Biological functions of inorganic elements. Biological ligands. Nucleotides and Nucleic acids (RNA, DNA) as ligands. Cobalamins including vitamin and co enzyme B12: Reactions of the alkylcobalamines, One electron and reduction and oxidation, activity of coenzyme B12, Metals at the center of photosynthesis: Magnesium and Manganese, Light absorption, Charge separation and electron transport. The oxygen molecule: Oxygen transport and storage through Hemoglobin and Myoglobin, Alternative oxygen transport in some lower animals: Hemerythin and Hemocyanin. Catalysis through Hemo proteins:

Electron transfer oxygen activation and Metabolism of Inorganic Intermediates. Cytochromes, cytochrome P-450: oxygen transfer from $O_2$ to non-activated substrates. Hemeproteins in the partially reduced nitrogen and sulfur compounds. Iron sulfur and other non heme Iron proteins: Biological relevance of the element combination Iron/sulfur. Rubredoxins, Ferredoxins, Polynuclear Iron sulfur clusters: Model systems for iron-sulfur proteins. Mononuclear nonheme iron enzymes. Transport and storage of an essential elements: The problem of iron mobilization, oxidation states, Iron uptake by plants. Transport and storage of iron, Ferritin, Hemosiderin: Biological function of the early transition metals: Enzymes containing the molybdenum cofactor. Metalo-enzymes in biological nitrogen cycle.

**Chem 6112 Colloidal and Nano-chemistry**

3.00 Credits, 3 hours/week

Methods of preparation, classification and general properties of colloids. Electrokinetic phenomena: Double layer structure, Zeta potential, electrophoresis and electroosmosis. Properties of gels and colloidal electrolytes. Preparation, types, specific properties and stability of emulsions. Micelles formation and critical micelle concentration.Uses of colloids, emulsions, and gels. Fundamental aspects of nanoscience and nanotechnology, fabrication method of nanomaterials: top down and bottom up process, chemical synthesis and modification of nanomaterials. Energy at the nanoscale: surface energy, basic thermodynamics, liquid state, surface energy minimization mechanism. Chemical interactions at the nanoscale: electrostatic interactions, hydrogen bonding, Van der Waals interaction and hydrophobic effect. Tools for nano characterizations: electron microscopy, atomic probe microscopy, X-ray spectroscopy, Raman spectroscopy, and Nanolithography. Advanced materials: fullerenes, carbon nanotubes, and diamondoids. Chemistry of nanoelectronics, nanophotonics, nanofluidics and nanobiotechnology. Nanotechnology products and applications. Societal implication of nano: ethical implications, legal implications, environmental implications, public perception.

**Chem 6113 Textile Chemistry**

3.00 Credits, 3 hours/week

Chemistry of Dyes and Color: Theories color formation, classification of dyes based on application and chemical constituents, synthesis of some common dyes used in textile industries. Textile fiber chemistry: Natural fiber, man-made fiber, synthetic fiber, chemical structure of cotton, Linen, cellulose, acrylic, wool, silk, nylon, polyester etc, chemical synthesis of synthetic dyes, Characterization of Structure of Fiber Forming Polymers. Finishing of fibers: Use of selective finishing agent/auxiliaries to modify fiber performance including oxidizing, softening and cross- linking agents, fiber aging-effect of heat, chemical and weather conditions on fiber structure and properties, Description and discussion of special finishing processes including water- repellency, easy- care finishing, flame retardancy, oil repellency, softening, anti- microbial finishing, chemical formulation used in these finishing effects, and their effects on fabric performance. Nanotechnology in textile: NanoTechnology in high performance textile, NanoTechnology in textile finishing, some selected application of nanotechnology in Textile. Medical textile: Textile medical products, bio-medical textile materials. Textile waste

management: Wastes in textile industries, removal of dyes and pigments from waste water, removal of toxic elements used in textile finishing.

**Chem 6114 Chemistry of Materials**

3.00 Credits, 3 hours/week

Concept and design of organic, inorganic and biomaterials. Types of chemical bonding in solid; ionic solids, metallic solids, covalent network solids, molecular solids.Crystalline state; crystal growth techniques, physical properties of crystal, bonding in crystalline solids. Amorphous state; sol-gel processing, cementitious materials. Properties, synthesis and structure-property relationship of metal, semiconductor, softmaterials and biomaterials. Materials characterization: optical microscopy, electron microscopy, scanning electron microscopy, scanning probe microscopy, NMR in material chemistry. Chemical approach for the design of fluids.

**Chem 6115 Advanced Photochemistry**

3.00 Credits, 3 hours/week

Photochemistry and radiation chemistry. Mechanism of dark reactions and photochemical reactions. Dosimeters. Basic principle of laser action, various types of lasers. flash photolysis, techniques in laser photochemistry, pico- and femtosecond photolysis, detection of short-lived species. Laser induced breakdown spectroscopy (LIBS), solar energy and solar simulation. Photochemical kinetics, excited species and their fates, photochemical quenching, photochemical processes in atmosphere, Stern-Volmer equation, photolysis. Photoelectrodes, types of photoelectrochemical solar cells, mechanism of energy conversion, energy conversion efficiency. Organic solar cells. Photoelectrochemical production of hydrogen from water. Storage of solar energy. Photocatalysts, Semiconducting metal oxides, Influence of photocatalysts on TOC and BOD of the dye effluents, Degradation of dyes and other organic substances in aqueous system. Roles of mediators, Kinetics of photodegradation of dyes in aqueous solution. Mechanism of advanced oxidation processes (AOP's) in water treatment: The hydrogen peroxide/ultraviolet light ($H_2O_2$/UV), ozone/ultraviolet light($O_3$/UV), hydrogen peroxide/Ozone(($H_2O_2$ /$O_3$), hydrogen peroxide/ultraviolet light/ozone ($H_2O_2$/$O_3$/UV), $TiO_2$/UV and $TiO_2$/UV + $H_2O_2$ processes.

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