

# Madhabdev University

(A State University Established under the Assam Act. No. XXXV of 2017)



## Curriculum and Syllabus Of Four Year Undergraduate Programme In Chemistry (Major)

From Academic Session  
2026-2027

**Department of Chemistry**  
**Narayanpur, P.O.: Dikrong (784164), Dist.: Lakhimpur, Assam**

## Course Distribution

| Sem  | Paper       | Paper Name                                                     | Paper Code | Marks Distribution |             | Credit Distribution |           | Total credit |
|------|-------------|----------------------------------------------------------------|------------|--------------------|-------------|---------------------|-----------|--------------|
|      |             |                                                                |            | In-Sem             | End-Sem     | Theory              | Practical |              |
| I    | Major I     | Core Chemistry- I                                              | CHMM-101   | 30                 | 70          | 4                   | 0         | 4            |
|      | Minor I     | General Chemistry- I                                           | CHMN-101   | 30                 | 70          | 4                   | 0         | 4            |
|      | SEC I       | Safety Measures and Standard Operation in Chemistry Laboratory | CHMS-101   |                    |             | 0                   | 3         | 3            |
|      | MDC I       | Chemistry in everyday life-I                                   | CHMD-101   |                    |             | 3                   | 0         | 3            |
|      | VAC I       |                                                                |            |                    |             | 2                   | 0         | 2            |
|      | AEC I       |                                                                |            |                    |             | 4                   |           | 4            |
|      |             |                                                                |            |                    | Total       | 17                  | 3         | 20           |
| II   | Major II    | Core Chemistry- II                                             | CHMM-201   | 30                 | 70          | 4                   | 0         | 4            |
|      | Minor II    | General Chemistry-II                                           | CHMN-201   | 30                 | 70          | 4                   | 0         | 4            |
|      | SEC II      | Basic analytical Chemistry                                     | CHMS-201   |                    |             | 0                   | 3         | 3            |
|      | MDC II      | Chemistry in everyday life-II                                  | CHMD-201   |                    |             | 3                   | 0         | 3            |
|      | VAC II      | IKS and Chemistry                                              | CHMV-201   |                    |             | 2                   | 0         | 2            |
|      | AEC II      |                                                                |            |                    |             | 4                   |           | 4            |
|      |             |                                                                |            |                    | Total       | 17                  | 3         | 20           |
| III  | Major III   | Core Chemistry- III                                            | CHMM-301   | 30                 | 70          | 4                   | 0         | 4            |
|      | Major IV    | Core Chemistry Practical-I                                     | CHMM-302   | 30                 | 70          | 0                   | 4         | 4            |
|      | Minor III   | General Chemistry-III                                          | CHMN-301   | 30                 | 70          | 4                   | 0         | 4            |
|      | SEC III     | Chemistry in Forensic Science                                  | CHMS-301   |                    |             | 1                   | 2         | 3            |
|      | MDC III     | Chemistry in everyday life-III                                 | CHMD-301   |                    |             | 3                   | 0         | 3            |
|      | VAC III     |                                                                |            |                    |             | 2                   | 0         | 2            |
|      |             |                                                                |            |                    | Total       | 14                  | 6         | 20           |
| IV   | Major V     | Inorganic Chemistry I                                          | CHMM-401   | 30                 | 70          | 4                   |           | 4            |
|      | Major VI    | Organic Chemistry I                                            | CHMM-402   | 30                 | 70          | 4                   | 0         | 4            |
|      | Major VII   | Physical Chemistry I                                           | CHMM-403   | 30                 | 70          | 4                   | 0         | 4            |
|      | Major VIII  | Organic Chemistry Practical                                    | CHMM-404   |                    |             | 0                   | 4         | 4            |
|      | Minor IV    | General Chemistry- IV (Practical)                              | CHMN-401   | 30                 | 70          | 0                   | 4         | 4            |
|      |             | Internship                                                     |            |                    |             | 0                   | 2         | 2            |
|      |             |                                                                |            |                    | Total       | 12                  | 8         | 22           |
| V    | Major IX    | Inorganic Chemistry II                                         | CHMM-501   | 30                 | 70          | 4                   |           | 4            |
|      | Major X     | Organic Chemistry II                                           | CHMM-502   | 30                 | 70          | 4                   | 0         | 4            |
|      | Major XI    | Physical Chemistry II                                          | CHMM-503   | 30                 | 70          | 4                   | 0         | 4            |
|      | Major XII   | Physical Chemistry Practical                                   | CHMM-504   |                    |             | 0                   | 4         | 4            |
|      | Minor V     | General Chemistry- V                                           | CHMN-501   | 30                 | 70          | 4                   | 0         | 4            |
|      |             | Internship                                                     |            |                    |             | 0                   | 2         | 2            |
|      |             |                                                                |            |                    | Total       | 16                  | 6         | 22           |
| VI   | Major XIII  | Inorganic Chemistry III                                        | CHMM-601   | 30                 | 70          | 4                   |           | 4            |
|      | Major XIV   | Organic Chemistry III                                          | CHMM-602   | 30                 | 70          | 4                   | 0         | 4            |
|      | Major XV    | Physical Chemistry III                                         | CHMM-603   | 30                 | 70          | 4                   | 0         | 4            |
|      | Major XVI   | Inorganic Chemistry Practical                                  | CHMM-604   |                    |             | 0                   | 4         | 4            |
|      | Major XVII  | Dissertation                                                   |            |                    |             | 0                   | 2         | 2            |
|      | Minor VI    | General Chemistry-VI                                           | CHMN-601   | 30                 | 70          | 4                   | 0         | 4            |
|      |             |                                                                |            |                    | Total       | 16                  | 6         | 22           |
| VII  | Major XIII  | Advanced Inorganic Chemistry I                                 | CHMM-701   | 30                 | 70          | 4                   |           | 4            |
|      | Major XIV   | Advanced Organic Chemistry I                                   | CHMM-702   | 30                 | 70          | 4                   | 0         | 4            |
|      | Major XV    | Advanced Physical Chemistry I                                  | CHMM-703   | 30                 | 70          | 4                   | 0         | 4            |
|      | Major XVI   | Research Methodology for Natural Sciences                      | CHMM-704   | 30                 | 70          | 3                   | 1         | 4            |
|      | Major XVII  | Dissertation/Advanced Practical I                              | CHMM-705   | 30                 | 70          | 0                   | 2         | 2            |
|      | Minor VII   | General Chemistry-VII (Practical)                              | CHMN-701   | 30                 | 70          | 0                   | 4         | 4            |
|      |             |                                                                |            |                    | Total       | 15                  | 7         | 22           |
| VIII | Major XVII  | Advanced Inorganic Chemistry II                                | CHMM-801   | 30                 | 70          | 4                   |           | 4            |
|      | Major XVIII | Advanced Organic Chemistry II                                  | CHMM-802   | 30                 | 70          | 4                   | 0         | 4            |
|      | Major XIX   | Advanced Physical Chemistry II                                 | CHMM-803   | 30                 | 70          | 4                   | 0         | 4            |
|      | Major XX    | Dissertation/Advanced Practical II                             | CHMM-804   |                    |             | 0                   | 8         | 4/8          |
|      | Minor VIII  | General Chemistry-VIII                                         | CHMN-801   | 30                 | 70          | 4                   | 0         | 4            |
|      |             |                                                                |            |                    | Total       | 16                  | 8         | 20/24        |
|      |             |                                                                |            |                    | Grand Total |                     |           | 174          |

## PART 1: OVERVIEW

### 1.1 Introduction

The National Education Policy 2020 (NEP 2020) presents a transformative vision for India's education system, aligned with the constitutional ideals of democracy, justice, equality, liberty, fraternity, and social responsibility. It seeks to reform every aspect of education, including its governance, regulation, curriculum, and institutional framework, to meet the evolving demands of the twenty-first century. The policy is also aligned with the objectives of the United Nations Sustainable Development Goal 4 (SDG 4), which aims to ensure inclusive, equitable, and quality education while promoting lifelong learning opportunities. At the same time, NEP 2020 emphasizes preserving India's rich cultural heritage and value systems. Its overarching objective is to nurture competent, creative, ethical, and socially responsible individuals who can contribute meaningfully to national and global development.

A key feature of NEP 2020 is its strong advocacy for multidisciplinary and holistic education. The policy recognizes that integrating the humanities, arts, and social sciences with Science, Technology, Engineering, and Mathematics (STEM) enriches the learning experience and fosters creativity, innovation, critical thinking, analytical reasoning, effective communication, teamwork, and problem-solving abilities. Such an interdisciplinary approach also enhances students' social awareness, ethical values, and overall engagement with learning, preparing them to address complex real-world challenges.

Recognizing research and innovation as fundamental drivers of national progress, NEP 2020 emphasizes the need to strengthen India's research ecosystem across all academic disciplines. It advocates expanding research opportunities and promoting innovation to transform India into a global knowledge hub. Within postgraduate education, the policy proposes a flexible curriculum that enables learners to pursue interdisciplinary studies while developing advanced subject knowledge, research aptitude, and professional competencies. This approach aims to equip graduates with the expertise and innovative mindset required to contribute to the vision of an *Atmanirbhar Bharat*, particularly in science, technology, and allied fields.

In accordance with the reforms introduced in undergraduate education, the Curriculum and Credit Framework for the Postgraduate Programme in Chemistry has been developed in line with the University Grants Commission (UGC) *Curriculum and Credit Framework for Postgraduate Programmes (2024)*. The framework adopts a learner-centric approach by incorporating a flexible Choice-Based Credit System (CBCS), multidisciplinary learning opportunities, and multiple entry and exit options. This structure empowers students to personalize their academic journey according to their interests, career aspirations, and research goals while promoting academic mobility and lifelong learning.

While preparing the syllabus, due consideration has been given to the evolving needs of students, educators, industry, and society. Each course clearly defines its learning outcomes, instructional strategies, assessment methods, and learning resources to facilitate effective knowledge acquisition and skill development. Beyond disciplinary expertise, the programme seeks to cultivate essential graduate attributes, including scientific temperament, ethical values, emotional resilience, critical and analytical thinking, social responsibility, environmental consciousness, and professional competencies. These qualities are expected to enhance students' employability while preparing them for advanced research, innovation, and meaningful contributions to society.

## 1.2 Bearings of NEP 2020 on the Curricula

The National Education Policy (NEP) 2020 envisions an education system deeply rooted in India's cultural heritage and value systems while responding effectively to the aspirations of a rapidly evolving global society. The policy aims to transform India into an equitable, inclusive, and vibrant knowledge society by ensuring access to high-quality education for all, thereby positioning the nation as a global leader in knowledge creation and innovation. It emphasizes the development of curricula and pedagogical practices that foster respect for the Fundamental Duties and Constitutional values, strengthen national identity, and cultivate an awareness of individual responsibilities in an interconnected and changing world. The policy seeks to nurture learners who take pride in India's rich cultural legacy while possessing the knowledge, skills, ethical values, and attitudes required to promote human rights, sustainable development, environmental stewardship, and global well-being as responsible global citizens.

To achieve these objectives, NEP 2020 identifies several guiding principles that are reflected in the design and implementation of higher education curricula:

- *Holistic Development: Recognize and nurture the unique abilities, interests, and potential of every learner to support their intellectual, emotional, ethical, and professional growth.*
- *Flexibility in Learning: Provide flexible curricular structures that enable students to choose learning pathways, interdisciplinary courses, and career trajectories aligned with their interests and aspirations.*
- *Promote an integrated approach to learning by encouraging interactions among the sciences, social sciences, arts, humanities, and other disciplines to address complex real-world challenges.*
- *Foster deep conceptual learning, analytical reasoning, creativity, innovation, and problem-solving abilities rather than rote memorization, while strengthening ethical values, constitutional principles, communication, teamwork, leadership, and resilience.*
- *Encourage the effective integration of digital technologies in teaching, learning, assessment, and academic administration to enhance accessibility, inclusivity, and learning outcomes, including support for Divyang learners.*
- *Ensure that curricula and pedagogy reflect India's linguistic, cultural, regional, and social diversity while addressing local and global needs*
- *Promote an inclusive learning environment that provides equitable access to quality education and supports learners from diverse backgrounds to achieve their full academic potential.*
- *Instil appreciation for India's rich heritage, indigenous knowledge systems, languages, traditions, and cultural diversity while preparing students to contribute effectively to national development and the global knowledge economy.*

## 1.3 Initiatives that Have a Bearing on Undergraduate Education

The National Education Policy (NEP) 2020 proposes a comprehensive transformation of higher education through learner-centric, multidisciplinary, and flexible academic frameworks that

promote holistic development, innovation, and lifelong learning. The key initiatives envisioned under the policy include:

- *Introduction of multidisciplinary undergraduate programmes that foster the intellectual, social, emotional, ethical, aesthetic, and physical development of learners while promoting critical thinking, creativity, communication, problem-solving, and disciplinary expertise.*
- *Adoption of flexible curricular structures that enable students to combine disciplines, choose elective courses across domains, and pursue personalised learning pathways according to their interests, abilities, and career aspirations.*
- *Implementation of undergraduate programmes of three or four years with multiple entry and exit provisions, allowing the award of*
  - ✓ UG Certificate after successful completion of one year (two semesters);
  - ✓ UG Diploma after two years (four semesters);
  - ✓ Bachelor's Degree after three years (six semesters); and
  - ✓ Bachelor's Degree with Honours after four years (eight semesters), or Bachelor's Degree with Honours and Research upon successful completion of a research project during the fourth year.
- *Recognition of the four-year undergraduate programme as the preferred pathway, providing students with greater opportunities for multidisciplinary learning, research exposure, and specialization through major and minor disciplines.*
- *Integration of credit-bearing courses and projects related to community engagement, environmental education, value-based education, internships, and experiential learning to promote social responsibility and practical competence.*
- *Encouragement of student participation in community service and outreach activities as an integral component of holistic education and experiential learning.*
- *Provision of opportunities for industrial internships, community-based learning, and research internships with faculty members, research institutions, industries, and other organizations to strengthen practical skills, research aptitude, and employability.*
- *Reorientation of academic programmes to encourage interdisciplinary learning by integrating the sciences, social sciences, humanities, languages, arts, vocational education, and sports, thereby creating a stimulating and inclusive learning environment.*
- *Incorporation of contemporary and emerging fields such as Nanotechnology, and other advanced technologies into higher education curricula to enhance innovation, research capability, and employability in alignment with national and global priorities.*

## PART 2: CURRICULUM & CREDIT FRAMEWORK

### 2.1 Eligibility

Applicants must have passed the Senior Secondary School Leaving Certificate (10+2) or Higher Secondary (Class XII) Examination, or an equivalent qualification corresponding to National Credit Framework (NCrF) Level 4.0, with **Chemistry** and preferably Mathematics as regular subjects.

### 2.2 Duration

The Undergraduate (UG) programme shall be of four years (eight semesters) in duration with multiple entry and exit options, in accordance with the provisions of the National Education Policy (NEP) 2020 and the UGC Curriculum and Credit Framework. Appropriate academic qualifications shall be awarded upon the successful completion of the prescribed credit requirements at each exit level.

Students may take a break from their studies during the programme. However, the maximum period permitted for completing all the requirements of the UG programme shall not exceed seven years from the date of initial admission.

### 2.3 UG Certificate, UG Diploma, and Degrees

#### 2.3.1 UG Certificate

A student who exits the Undergraduate (UG) programme after successfully completing the first year (two semesters) and fulfilling the prescribed credit requirements shall be awarded a UG Certificate in Chemistry. Such students may re-enter the programme within three years from the date of exit to complete the remaining requirements for the Bachelor's degree, in accordance with the institutional regulations and the provisions of the NEP 2020 and the UGC Curriculum and Credit Framework.

#### 2.3.2 UG Diploma

A student who exits the Undergraduate (UG) programme after successfully completing the second year (four semesters) and fulfilling the prescribed credit requirements shall be awarded a UG Diploma in Chemistry. Students who exit with a UG Diploma may re-enter the programme within three years from the date of exit to complete the remaining requirements for the Bachelor's degree, in accordance with the institutional regulations and the provisions of the NEP 2020 and the UGC Curriculum and Credit Framework.

#### 2.3.3 3-Year Bachelor's Degree (Major)

A student who successfully completes the third year (six semesters) of the Undergraduate (UG) programme and fulfils the prescribed credit requirements shall be awarded a Bachelor's Degree (Major) in Chemistry.

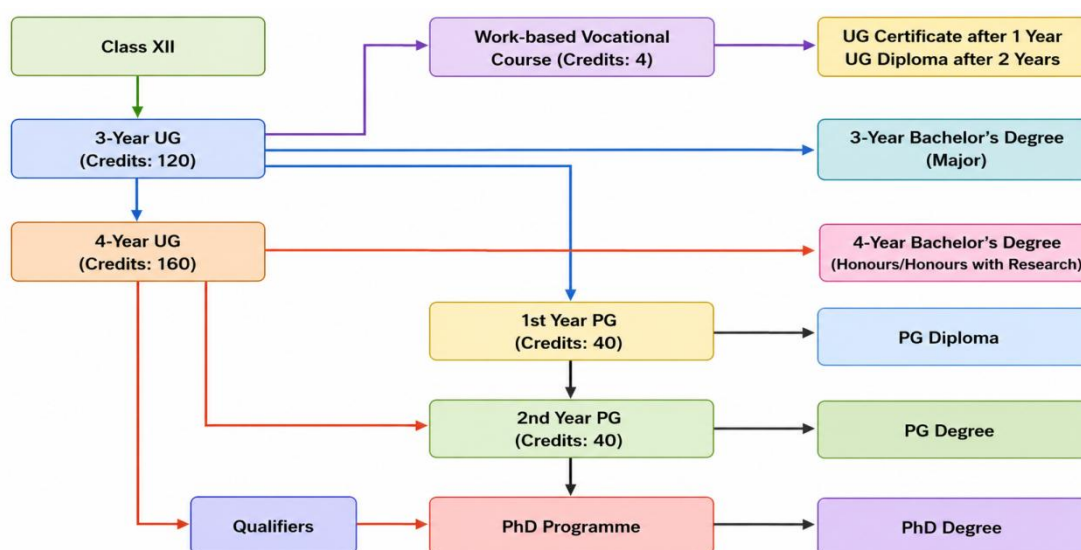
#### 2.3.4 4-Year Bachelor's Degree (Honours)

A student who successfully completes the fourth year (eight semesters) of the Undergraduate (UG) programme and fulfils the prescribed credit requirements shall be awarded a Bachelor's Degree (Honours) in Chemistry.

### 2.3.5 4-Year Bachelor's Degree (Honours with Research)

A student who successfully completes the fourth year (eight semesters) of the Undergraduate (UG) programme and fulfils the prescribed credit requirements shall be awarded a Bachelor's Degree (Honours) in Chemistry.

## 2.4 Progression of PG Programmes in Chemistry



### 2.5 Nature and Extent of the Four-Year Undergraduate Programme in Chemistry

The Four-Year Undergraduate Programme (FYUP) in Chemistry is designed to provide students with a strong foundation in the core areas of Inorganic, Organic, Physical, Analytical, and Materials Chemistry, while introducing them to emerging and interdisciplinary fields. The curriculum comprises well-structured courses with clearly defined objectives, learning outcomes, and assessment strategies, enabling students to acquire comprehensive theoretical knowledge, practical skills, and scientific competencies. The availability of elective courses allows students to explore areas of personal interest and broaden their expertise in chemistry and allied disciplines.

The programme integrates contemporary interdisciplinary subjects such as Nanomaterials, Biomaterials, Environmental Chemistry, Green Chemistry, and Materials Chemistry, highlighting their applications in modern science and technology. By establishing strong linkages between chemistry and related disciplines such as Physics, Biology, Mathematics, Environmental Science, and Materials Science, the curriculum promotes multidisciplinary learning and research. The inclusion of frontier areas of chemistry enhances students' conceptual understanding, laboratory skills, and research aptitude, preparing them to meet the evolving needs of academia, research institutions, and the chemical and allied industries.



The curriculum is also designed to prepare students for national-level competitive examinations, higher education, and research opportunities. In accordance with the holistic and multidisciplinary vision of NEP 2020, students have the flexibility to choose courses from allied disciplines such as Physics, Mathematics, Biology, and Ability Enhancement Courses (AECs) to complement their major programme. Equal emphasis is placed on developing employability by strengthening students' theoretical knowledge, practical competence, digital proficiency, and problem-solving abilities. In addition, the programme incorporates Skill Enhancement Courses (SECs) and experiential learning components to equip graduates with professional, technical, and entrepreneurial skills required for careers in industry, research, academia, and other allied sectors.

## 2.6 Programme Educational Objectives (PEOs)

The Four-Year Undergraduate Programme (FYUP) in Chemistry aims to achieve the following Programme Educational Objectives (PEOs):

- PEO 1:** Develop a comprehensive understanding of the fundamental principles, theories, concepts, and applications of chemistry, with a strong foundation in inorganic, organic, physical, analytical, and materials chemistry.
- PEO 2:** Equip students with analytical, critical thinking, and problem-solving skills to address theoretical, experimental, and real-world challenges in chemistry using appropriate scientific methods.
- PEO 3:** Prepare students for higher education, multidisciplinary research, entrepreneurship, and professional careers by developing advanced knowledge, practical skills, innovation, and scientific competence relevant to academia, industry, and self-employment.
- PEO 4:** Foster holistic intellectual development by providing a learner-centric environment that promotes scientific inquiry, conceptual understanding, ethical reasoning, creativity, and an appreciation of the role of chemistry in addressing societal and environmental challenges.
- PEO 5:** Strengthen students' theoretical knowledge, laboratory skills, research aptitude, and technical competencies through exposure to contemporary developments, modern instrumentation, computational tools, and experiential learning, enabling them to pursue higher studies and professional careers in chemistry and allied disciplines.
- PEO 6:** Develop responsible, ethical, and socially conscious graduates with effective communication, leadership, teamwork, critical thinking, lifelong learning, and constitutional values, empowering them to contribute meaningfully to society and sustainable development.

## 2.7 Programme Outcomes (POs)

|  | Type of PO | Programme Outcome (PO) Descriptor |
|--|------------|-----------------------------------|
|--|------------|-----------------------------------|



|      |                                          |                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
|------|------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| PO 1 | Problem Solving                          | Graduates will be able to identify, analyse, and solve familiar and unfamiliar theoretical, experimental, and real-life problems by applying the fundamental principles of chemistry, scientific reasoning, and appropriate analytical techniques. They will make informed decisions and develop effective solutions using critical thinking and evidence-based approaches.                                                                      |
| PO 2 | Analytical Reasoning & Critical Thinking | Graduates will demonstrate the ability to critically analyse scientific concepts, evaluate experimental evidence, interpret data, identify assumptions and logical inconsistencies, synthesize information from diverse sources, and formulate well-reasoned conclusions supported by scientific evidence.                                                                                                                                       |
| PO 3 | Creativity & Innovation                  | Graduates will apply creativity and innovation to address complex chemical problems by generating original ideas, exploring multiple perspectives, and developing sustainable and practical solutions. They will demonstrate imaginative thinking, adaptability, teamwork, and emotional intelligence while contributing effectively to scientific research, industry, and society.                                                              |
| PO 4 | Communication Skills                     | Graduates will communicate scientific concepts, experimental findings, and technical information effectively through oral, written, and digital media. They will critically evaluate scientific literature, prepare reports and presentations, construct logical arguments using appropriate chemical terminology, and communicate professionally with diverse audiences while demonstrating respect for cultural, gender, and social diversity. |
| PO 5 | Research- Related Skills                 | Graduates will develop research aptitude by identifying scientific problems, formulating research questions and hypotheses, designing and conducting experiments, analysing and interpreting data using appropriate methodologies and statistical tools, and communicating research findings while adhering to ethical principles and good scientific practices.                                                                                 |
| PO 6 | Collaboration and Teamwork               | Graduates will work effectively as individuals and as members of multidisciplinary teams by demonstrating cooperation, mutual respect, interpersonal skills, and shared responsibility in achieving common academic, research, and professional goals.                                                                                                                                                                                           |
| PO 7 | Leadership Development                   | Graduates will demonstrate leadership qualities by planning, organizing, and coordinating academic and professional activities, motivating team members, making informed decisions, and managing resources effectively to achieve organizational and societal objectives.                                                                                                                                                                        |

|       |                                                |                                                                                                                                                                                                                                                                                                                                                                                                       |
|-------|------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| PO 8  | Digital and Technological Skills               | Graduates will effectively utilize digital technologies, information and communication technology (ICT), scientific databases, computational tools, and discipline-specific software for data acquisition, analysis, visualization, scientific communication, and problem-solving in chemistry and related fields.                                                                                    |
| PO 9  | Multicultural Competence and Inclusive Spirit  | Graduates will demonstrate respect for cultural diversity, inclusivity, and global perspectives by working effectively in multicultural environments. They will exhibit empathy, gender sensitivity, social responsibility, and the ability to collaborate with diverse groups while promoting equality, inclusiveness, and mutual respect.                                                           |
| PO 10 | Value Inculcation                              | Graduates will uphold constitutional values, professional ethics, scientific integrity, and universal human values in their personal and professional lives. They will demonstrate honesty, accountability, respect for intellectual property rights, ethical decision-making, and responsible citizenship while addressing societal and global challenges through sustainable and ethical practices. |
| PO 11 | Environmental Awareness and Sustainability     | Graduates will apply scientific knowledge and environmental ethics to promote sustainable development, environmental conservation, pollution control, waste management, biodiversity conservation, and responsible utilization of natural resources. They will actively contribute to addressing environmental challenges, including climate change and ecological sustainability.                    |
| PO 12 | Community Engagement and Social Responsibility | Graduates will actively participate in community engagement, outreach programmes, and extension activities by applying chemical knowledge and scientific skills to address societal needs. They will contribute to public welfare, environmental awareness, health, and sustainable community development through responsible and ethical practices.                                                  |

## 2.8 Programme Specific Outcomes (PSOs)

|       | Type of PSO               | Programme Specific Outcome (PSO) Descriptor                                                                                                                                                                                                                                                                                                                                                                                    |
|-------|---------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| PSO 1 | Knowledge & Understanding | Graduates will acquire a strong foundation in the theoretical and practical aspects of Analytical, Inorganic, Organic, Physical, Materials, and Environmental Chemistry, along with an understanding of emerging interdisciplinary areas. They will apply chemical principles and concepts to solve scientific problems and appreciate the role of chemistry in addressing societal, industrial, and environmental challenges. |

|       |                                                      |                                                                                                                                                                                                                                                                                                                                                                                                                      |
|-------|------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| PSO 2 | Discipline-Specific Skills                           | Graduates will develop proficiency in laboratory techniques, chemical synthesis, qualitative and quantitative analysis, instrumentation, computational tools, and data interpretation. They will be equipped with the scientific and technical skills necessary for higher studies, research, and professional careers in chemistry and allied disciplines.                                                          |
| PSO 3 | Application of Knowledge and Skills                  | Graduates will apply chemical concepts, experimental methodologies, and analytical approaches to design, perform, and interpret chemical syntheses, analyses, and investigations. They will utilize scientific knowledge to solve problems in chemistry and contribute effectively to multidisciplinary research, industrial applications, and sustainable technological development.                                |
| PSO 4 | Quantitative, Analytical and Instrument-based Skills | Graduates will acquire hands-on experience in classical quantitative analysis and modern analytical instrumentation. They will develop the competence to operate, maintain, and interpret data from sophisticated instruments, enabling them to work effectively in chemical, pharmaceutical, environmental, materials, forensic, food, and biochemical laboratories, as well as pursue higher studies and research. |

## 2.9 Structure of the Undergraduate Programme

The curriculum of the Four-Year Undergraduate Programme (FYUP) in Chemistry has been designed in accordance with the UGC Curriculum and Credit Framework for Undergraduate Programmes (2022). It aims to provide students with a comprehensive education that integrates disciplinary knowledge, practical skills, ethical values, research aptitude, and multidisciplinary learning in line with the objectives of NEP 2020.

The programme adopts a flexible and learner-centric structure comprising Major Courses, Minor Courses, Multidisciplinary Courses (MDC), Ability Enhancement Courses (AEC), Skill Enhancement Courses (SEC), Value Added Courses (VAC), Summer Internship/Apprenticeship, Research Project/Dissertation, and Community Engagement Activities. This framework enables students to acquire domain-specific expertise while developing interdisciplinary knowledge, professional competencies, and lifelong learning skills.

Students may review their academic interests after the second semester and, subject to institutional regulations, request a change in their chosen Major. The programme also provides opportunities to pursue Minor courses from other disciplines, thereby enhancing employability, multidisciplinary exposure, and career flexibility.

**2.9.1 Major Courses:** Major Courses constitute the primary component of the programme and are divided into Core Courses and Departmental Elective Courses.

**Core Courses:** Core Courses provide a strong foundation in the fundamental and advanced areas of Inorganic, Organic, Physical, Analytical, and Materials Chemistry. The courses progress from introductory to advanced levels, enabling students to develop a sound understanding of chemical concepts, theories, principles, and applications. Laboratory experiments, computational tools,

software-based learning, project work, and hands-on training with modern analytical instruments enhance students' practical skills, scientific reasoning, and research aptitude.

The minimum credit requirements for Major Courses are:

**3-Year Bachelor's Degree (Major):** 128 Credits

**4-Year Bachelor's Degree (Honours/ Honours with Research):** 174 Credits

**2.9.2 Minor Courses:** Minor Courses provide students with opportunities to acquire knowledge and skills in disciplines other than their Major. Students are encouraged to choose Minor Courses from cognate or other relevant disciplines to broaden their academic perspective and improve career prospects.

**2.9.3 Multidisciplinary Courses (MDC):** Multidisciplinary Courses are intended to broaden students' intellectual horizons by exposing them to disciplines outside their Major and Minor areas of study. Each student shall complete three introductory-level MDCs (9 credits) selected from approved subject groups.

Students shall not choose MDCs from subjects already studied at the Higher Secondary (Class XII) level if those subjects are part of their Major or Minor.

**2.9.4 Ability Enhancement Courses (AEC):** Ability Enhancement Courses are designed to strengthen students' communication and language proficiency. These compulsory courses focus on English and a Modern Indian Language (MIL) to develop effective reading, writing, speaking, listening, and presentation skills required for academic and professional success. Students shall complete 8 credits under this category.

**2.9.5 Skill Enhancement Courses (SEC):** Skill Enhancement Courses aim to develop practical, technical, digital, entrepreneurial, and soft skills through hands-on learning and experiential training. These compulsory courses enhance students' employability and prepare them for careers in academia, industry, entrepreneurship, and allied sectors. Students shall complete 9 credits under this category.

**2.9.6 Value Added Courses (VAC):** Value Added Courses promote holistic development by integrating knowledge, values, ethics, and life skills beyond disciplinary boundaries.

Students shall complete courses in the following areas:

Understanding India

Environmental Science

Digital and Technological Solutions

Health & Wellness, Yoga Education, Sports and Fitness

These courses carry a total of 6 credits.

The Environmental Science courses shall be offered in accordance with the UGC Guidelines and Curriculum Framework for Environment Education at the Undergraduate Level (2023). Courses under Understanding India may include Indian Knowledge Systems (IKS) with appropriate emphasis on the historical development and contributions of chemistry in ancient India.

**2.9.7 Summer Internship / Apprenticeship:** To strengthen experiential learning, every student shall undertake a Summer Internship or Apprenticeship carrying 2 credits. The internship may be completed in industries, research laboratories, academic institutions, government organizations, or other relevant organizations. Alternatively, students may undergo laboratory training under faculty

members or researchers within their institution or at other recognized higher educational institutions or research organizations.

Students may also undertake a Field-based Minor Project during the summer term to gain first-hand exposure to community issues, industrial practices, environmental challenges, or socio-economic development. Such projects encourage students to apply classroom knowledge to real-world situations and develop problem-solving, observational, and analytical skills.

**2.9.8 Research Project / Dissertation:** Students enrolled in the Four-Year Bachelor's Degree (Honours with Research) shall undertake a Research Project/Dissertation under the supervision of a faculty member during the eighth semester.

The research project aims to develop scientific inquiry, experimental design, data analysis, research ethics, and scientific communication. Research outcomes may be disseminated through publications in peer-reviewed journals, presentations at conferences or seminars, or patent applications, subject to the originality and quality of the work.

**2.9.9 Community Engagement and Other Activities:** Students are encouraged to participate in National Service Scheme (NSS), National Cadet Corps (NCC), Unnat Bharat Abhiyan (UBA), adult education and literacy programmes, mentoring initiatives, environmental awareness campaigns, science outreach activities, and other community service programmes. Community engagement forms an integral component of holistic education and provides opportunities for students to understand societal challenges, apply scientific knowledge to address real-life problems, and contribute to sustainable development and nation-building. These activities also promote social responsibility, leadership, teamwork, ethical values, and experiential learning in accordance with the vision of NEP 2020.

## Semester I

|                              |                                                                          |
|------------------------------|--------------------------------------------------------------------------|
| <i>NCrF level</i>            | 4.5                                                                      |
| <i>Title of the Course</i>   | <i>Core Chemistry- I</i>                                                 |
| <i>Course code</i>           | <i>CHMM-101</i>                                                          |
| <i>Paper credit</i>          | 04 ((L 4 – T 0 - P 0)                                                    |
| <i>Total Contact Hours</i>   | <i>Theory 70</i>                                                         |
| <i>Distribution of Marks</i> | <i>Theory 100 (End semester examination 70 + internal assessment 30)</i> |

### Course Objectives

By the end of this course, students will be able to:

- Understand the historical development of atomic structure from classical mechanics to quantum mechanics and explain the quantum mechanical description of atoms and electronic configurations.
- Explain periodic trends in the physical and chemical properties of elements and relate these trends to electronic structure and effective nuclear charge.
- Understand the electronic effects governing the structure, stability, and reactivity of organic molecules and explain the formation, stability, and behaviour of reactive intermediates and apply thermodynamic and kinetic principles to interpret organic reaction mechanisms.
- Develop a sound understanding of stereochemistry, including molecular chirality, stereochemical nomenclature, and conformational analysis of organic molecules.
- Apply the kinetic theory of gases and equations of state to explain the behaviour of ideal and real gases under different physical conditions.
- Develop scientific reasoning, quantitative problem-solving ability, and analytical skills by integrating concepts from inorganic, organic, and physical chemistry.

### Course Outcomes (COs)

After successful completion of this course, the students will be able to:

- CO1.** Explain the evolution of atomic theory from classical to quantum mechanics, Schrödinger wave equation, quantum numbers, and electronic configuration of atoms.
- CO2.** Interpret periodic trends in atomic and ionic properties based on electronic structure.
- CO3.** Analyse the influence of electronic effects on the stability, acidity/basicity, and reactivity of organic molecules and distinguish between electrophiles and nucleophiles.
- CO4.** Explain the formation, stability, and reactivity of organic reaction intermediates and analyse reaction pathways
- CO5.** Apply stereochemical principles to represent, identify, and classify stereoisomers using various projection formulae and evaluate conformational stability of organic compounds.
- CO6.** Apply the kinetic molecular theory, Maxwell–Boltzmann distribution, van der Waals equation, virial equation, and related gas laws to solve problems involving ideal and real gases.

**Unit I: Atomic Structure****Lecture/Marks: 20**

Classical mechanics: Newtonian mechanics, wave concept and electromagnetic theory of radiation, inadequacy of classical mechanics: Black body radiation and laws associated, photoelectric effect, Compton Effect, discrete energy levels, Bohr's theory of structure of atom, hydrogen atom spectrum, wave particle duality and its experimental confirmation, uncertainty principle and its basis

Mathematical description of waves, Schrodinger time independent wave equation, concept of wave function, properties of wave function, normalised and orthogonal wave functions, Eigen function, Significance of  $\Psi$  and  $\Psi^2$

Schrodinger equation of hydrogen atom (no derivation), radial and angular wave functions probability distribution functions, representation of orbitals, the quantum numbers

Many electron atoms: Effective nuclear charge, Slater's Rule, Sequence of energy levels, electronic configuration, Aufbau's principle, Pauli's Exclusion Principle, Hund's rule, stability of half-filled and fully filled subshells (exchange energy).

**Unit II: Periodicity in Properties of atoms and ions****Lecture/Marks: 05**

General trends of the following properties across the period and down the group: electronic configurations and types of elements, Melting and boiling points, Density, atomic radius, van der Waals radius, metallic radius, covalent and ionic radius, thermochemical radii, ionization energies, electron affinities, electronegativity (various scales), group electronegativity, Secondary periodicity, Relativistic Effect, Inert pair effect.

**Unit III: Basic Organic Chemistry****Lecture/Marks: 10**

Concept of Inductive, Electrometric, Resonance, mesomeric effects and hyperconjugation and their applications, Concept of electrophiles and nucleophiles, nucleophilicity and basicity

Basic ideas about different types of reactions: addition, substitution, elimination, rearrangement, and condensation reactions, rate constant and free energy of activation, energy profile diagrams for one-step and multi-step reactions, curly arrow rules, formal charges.

Concepts of aromatic, anti-aromatic and non-aromatic compounds, Hückel's rules for aromaticity up to [8] annulene (including mononuclear heterocyclic compounds up to 6-membered ring); concept of antiaromaticity and homoaromaticity; non-aromatic molecules, Frost diagram (qualitative drawing)

**Unit IV: Stereochemistry-I****Lecture Marks 15**

Representation of organic molecules: Fischer, saw-horse, Newman, and flying-wedge, projection formulae and their interconversion.

Concept of chirality and symmetry: Symmetry elements, molecular chirality, optical activity, optical purity, meso-compounds, racemic mixture, resolution, enantiomers, diastereomers, epimers, anomers, atropisomers

Basic concepts of stereochemical nomenclatures: threo/erythro, syn/anti, R/S, cis/trans and E/Z,  $\alpha/\beta$  and endo/exo epimers, anomers.

Conformation: conformational nomenclature: eclipsed, staggered, gauche, syn and anti; dihedral angle, torsion angle; Klyne-Prelog terminology; P/M descriptors; energy barrier of rotation, concept



of torsional and steric strains; relative stability of conformers on the basis of steric effect, dipole-dipole interaction and H-bonding; butane gauche interaction; conformational analysis of ethane, propane, n-butane, 2-methylbutane and 2,3-dimethylbutane; haloalkane, 1,2-dihaloalkanes and 1,2-diols (up to four carbons); 1,2-halohydrin; conformation of conjugated systems (s-cis and s-trans).

### Unit V: States of Matter-I (Gaseous State)

Lecture Marks 20

Kinetic Theory of Gases: Postulates and derivation of the kinetic gas equation; collision frequency; collision diameter; mean free path and viscosity of gases, including their temperature and pressure dependence, the relation between mean free path and coefficient of viscosity, calculation of  $\sigma$  from  $\eta$ ; variation of viscosity with temperature and pressure.

Real Gas behaviour and Its Deviations: Deviations from ideal gas behaviour, compressibility factor, Z, and its variation with pressure for different gases. Causes of deviation from ideal behaviour, van der Waals equation of state, its derivation and application in explaining real gas behavior, introduction of equations of state; virial equation of state; van der Waals equation expressed in virial form and calculation of Boyle temperature. Isotherms of real gases and their comparison with van der Waals isotherms, continuity of states, critical state, relation between critical constants and van der Waals constants, and law of corresponding states

Molecular Motion and Energy Distribution in Gases: Maxwell-Boltzmann Distribution of Molecular Speeds and Its Applications in Determining Average, Root Mean Square, and Most Probable Velocities; Average Kinetic Energy; Law of Equipartition of Energy; Degrees of Freedom; and Molecular Interpretation of Heat Capacities.

### Suggested reading

- *Quantum Chemistry including Spectroscopy*, B.K.Sen, 4<sup>th</sup> edition, Kalyani Publishers
- *Fundamentals of Quantum Chemistry*, P.K. Bhattacharyya, Global Publishing House (India)
- *General and Inorganic Chemistry*, R.P. Sarkar (part 1) 3<sup>rd</sup> edition, NCBA
- *Concise Inorganic Chemistry*, J. D. Lee, 5<sup>th</sup> Edition, Pearson Education
- *Morrison, R. N. & Boyd, R. N. Organic Chemistry*, 6<sup>th</sup> Edition, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- *H. Pine. Organic Chemistry*, 5<sup>th</sup> Edition, McGraw-Hill Book (1987)
- *P. S. Kalsi. Stereochemistry, Conformation and Mechanism* 3<sup>rd</sup> Edition, John Wiley (1995).
- *D. Nasipuri, Stereochemistry of Organic Compounds. Principles and Applications*, Second Edition, Wiley Eastern Limited, New Delhi, 1994.
- *Atkins, P. W.; de Paula, J.; Keeler, J., Physical Chemistry*, 11<sup>th</sup> Edition, Oxford University Press India (2018). (ISBN: 978-0198814740).
- *Puri, B. R.; Sharma, L. R.; Pathania, M. S., Principles of Physical Chemistry*, 47<sup>th</sup> Edition, Vishal Publishing (2020). (ISBN: 978-9382956013).
- *Kapoor, K. L., A Textbook of Physical Chemistry: States of Matter and Ions in Solution*, Vol. I, 6<sup>th</sup> Edition, McGraw Hill Education India (2019). (ISBN: 978-9353165185).
- *Bahl, A.; Bahl, B. S.; Tuli, G. D., Essentials of Physical Chemistry*, 28<sup>th</sup> Ed., S. Chand and Company (2020). (ISBN: 978-9352836093)

## Semester II

|                              |                                                                          |
|------------------------------|--------------------------------------------------------------------------|
| <i>NCrF level</i>            | 4.5                                                                      |
| <i>Title of the Course</i>   | <i>Core Chemistry- II</i>                                                |
| <i>Course code</i>           | <i>CHMM-201</i>                                                          |
| <i>Paper credit</i>          | <i>04 ((L 4 – T 0 - P 0)</i>                                             |
| <i>Total Contact Hours</i>   | <i>Theory 70</i>                                                         |
| <i>Distribution of Marks</i> | <i>Theory 100 (End semester examination 70 + internal assessment 30)</i> |

### Course Objectives

Upon successful completion of this course, students will be able to:

- Understand the fundamental principles of chemical bonding and explain molecular structure using various theories and models.
- Correlate the nature of chemical bonding and intermolecular interactions with the physical and chemical properties of molecules and solids.
- Develop a comprehensive understanding of coordination chemistry, including coordination compounds, nomenclature, bonding, and stereoisomerism.
- Understand the mechanisms, kinetics, stereochemistry, and selectivity of important organic reactions, including substitution, elimination, and aromatic substitution reactions.
- Explain the structure and properties of crystalline solids, liquids, liquid crystals, and colloidal systems using modern concepts of physical chemistry.
- Apply theoretical concepts from inorganic, organic, and physical chemistry to analyse chemical phenomena and solve qualitative and quantitative problems.

### Course Outcomes (COs)

After successful completion of this course, the students will be able to:

- CO1.** Explain chemical bonding using Lewis theory, VSEPR theory, Valence Bond Theory, Molecular Orbital Theory, and lattice energy models, and correlate bonding with molecular geometry, polarity, aromaticity, and intermolecular forces.
- CO2.** Analyse the bonding, nomenclature, stereochemistry, and isomerism of coordination compounds based on Werner's theory and modern coordination chemistry concepts.
- CO3.** Analyse the structure, stability, and reactivity of organic reaction intermediates and explain reaction mechanisms involving substitution, elimination, addition, rearrangement, electrophilic aromatic substitution, and nucleophilic aromatic substitution using thermodynamic and kinetic principles.
- CO4.** Explain the structure and properties of crystalline solids, crystal defects, band theory, and packing arrangements, and relate these concepts to the physical properties of materials.
- CO5.** Describe the physical properties of liquids, liquid crystals, and colloidal systems, explain their stability and behaviour, and apply the principles governing colloidal phenomena to chemical and industrial processes.

**Unit I Bonding Theories****Lecture/Marks: 20**

Electronic theory of Valency: octet rule, Lewis electron dot formula, formal charge, electroneutrality principle.

Shapes of molecules: Valence shell electron pair repulsion (VSEPR) theory (steric number, merits and demerits).

The chemical bond: Bond length, bond strength, bond angle, bond energy, polarity of bonds.

Valence Bond theory (VBT): The basic approach, some useful concept of VBT, Energetics of hybridization, equivalent and non-equivalent hybrid orbitals, Bent's rule, calculation of formal charges and double bond equivalent (DBE); orbital pictures of bonding ( $sp^3$ ,  $sp^2$ ,  $sp$ : C-C, C-N & C-O systems)

Molecular orbital theory (MOT): Introduction, linear combination of orbitals, types of molecular orbitals, MO diagrams of homonuclear (Li-Ne) and heteronuclear diatomic (HF, CO, NO,  $CN^-$ ), and HCl (idea of s-p mixing and orbital interaction), idea about  $\sigma$ ,  $\sigma^*$ ,  $\pi$ ,  $\pi^*$ , n – MOs; concept of HOMO, LUMO and SOMO; sketch and energy levels of  $\pi$  MOs of acyclic p orbital system (C=C, conjugated diene, triene, allyl and pentadienyl systems)

Covalent character in ionic compounds: polarising power and polarizability, Fajan's rules and consequences of polarisation.

Ionic character in covalent compounds: influence of hybridization on bond properties: bond dissociation energy (BDE) and bond energy; bond distances, bond angles; concept of bond angle strain, Bond dipole, dipole moment, and molecular polarizabilities, percentage ionic character.

Bonding models in ionic compounds: Properties of ionic substances, lattice and solvation energy; Born Lande equation; Kapustinski equation, Madelung constant, Born Haber Cycle for lattice energy calculation.

Weak Chemical Forces: van der Waals forces, ion-dipole forces, dipole-dipole interactions, induced dipole interactions, instantaneous dipole-induced dipole interactions and hydrogen bonding; melting point/boiling point and solubility of common organic compounds in terms of covalent & non-covalent intermolecular forces

**Unit II: Introduction to Coordination Chemistry****Lecture/Marks: 05**

Coordinate bonding; double and complex salts. Werner's theory of coordination complexes, Classification of ligands, Ambidentate ligands, chelates, Coordination numbers, IUPAC nomenclature of coordination complexes (up to two metal centers), Isomerism in coordination compounds, constitutional and stereo isomerism, Geometrical and optical isomerism in square planar and octahedral complexes

**Unit IV: Organic Reaction intermediate****Lecture/Marks: 10**

Reaction thermodynamics: Free energy and equilibrium, enthalpy and entropy factor, calculation of enthalpy change via BDE, intermolecular & intramolecular reactions.

Reaction kinetics: Rate constant and free energy of activation; free energy profiles for one-step, and two-step reactions; catalyzed reactions, principle of microscopic reversibility; Hammond's postulate.

Generation, structure and reactivity, classical and non-classical carbocations, neighboring group participation and rearrangements in acyclic, monocyclic and bicyclic systems, carbanions, carbon radicals: generation and stability, structure and electrophilic/nucleophilic behaviour of reactive intermediates like carbenes, nitrenes, Enolates (Thermodynamic versus kinetic enolates, enolate equivalent and enamines), Ylides (Chemistry of phosphorous and sulfur ylides, stabilized and non-stabilised ylides), Arynes (Generation, structure and stability, rearrangement reactions)

**Unit IV: Organic Reaction mechanism****Lecture/Marks: 10**

Nucleophilic Substitution at  $sp^3$  carbon centre mechanism: substitution at  $sp^3$  centre (systems: alkyl halides, allyl halides, benzyl halides, alcohols, ethers, epoxides,  $\alpha$ -halocarbonyls), mechanisms (with evidence), relative rates & stereochemical features:  $SN_1$ ,  $SN_2$ ,  $SN_2'$ ,  $SN_1'$  (allylic rearrangement) and  $SN_i$ ; effects of solvent, substrate structure, leaving group and nucleophiles (including ambident nucleophiles, cyanide & nitrite); substitutions involving NGP (with hetero atoms and aryl groups); role of crown ethers and phase transfer catalysts.

Elimination Reaction:  $E_1$ ,  $E_2$ ,  $E_1cB$  and  $E_i$  (pyrolytic syn eliminations); formation of alkenes and alkynes; mechanisms (with evidence), reactivity, regioselectivity (Saytzeff/Hofmann) and stereoselectivity; comparison between substitution and elimination.

Electrophilic aromatic substitution Mechanisms:  $\pi$ - and  $\zeta$ -complex, ipso substitution, activating and deactivating groups, orienting influence. Reactions: Friedel-Crafts alkylation/acylation, nitration, sulfonation, halogenation, formylation.

Nucleophilic Aromatic Substitution Mechanisms, orientation, and reactivity

#### **Unit VI: States of Matter-II (Solid state)**

**Lecture/Marks: 15**

General characteristics of solid state, amorphous and crystalline solids, classification of crystalline solids, crystal lattices and unit cells, number of atoms in unit cell, closed packed structures, radius ratio rule, voids, packing efficiency and calculations, imperfections in solids, electrical and magnetic properties. Examples of crystal structures: NaCl, CsCl, ZnS,  $CaF_2$ ,  $TiO_2$

Band theory of solids

Law of constancy of interfacial angles, crystal planes, law of rational indices, Miller indices, space lattice and unit cell, packing in crystals, crystal defects

#### **Unit VII: States of Matter-III (Liquid State)**

**Lecture/Marks 10**

Qualitative description of the structure of liquids, Physical properties of liquids - vapour pressure, surface tension, viscosity, Methods for determination of surface tension and viscosity, refractive index (definitions and descriptions), Liquid crystals- elementary discussion on structure and types of liquid crystals

#### **Suggested Readings**

- General and Inorganic Chemistry, R.P. Sarkar (part 1) 3rd edition, NCBA
- Inorganic Chemistry (Principles of Structure and Reactivity), J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, 5<sup>th</sup> edition, Pearson Education
- March, J., Smith, M. B. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6th Edn., (Wiley, 2007).
- P. S. Kalsi. Stereochemistry, Conformation and Mechanism (3rd edn.), John Wiley (1995).
- D. Nasipuri, Stereochemistry of Organic Compounds. Principles and Applications, Second Edition, Wiley Eastern Limited, New Delhi, 1994. Ch.2-6 and 9-12.
- Atkins, P. W.; de Paula, J.; Keeler, J., Physical Chemistry, 11th Ed., Oxford University Press India (2018). (ISBN: 978-0198814740).
- Puri, B. R.; Sharma, L. R.; Pathania, M. S., Principles of Physical Chemistry, 47th Ed., Vishal Publishing (2020). (ISBN: 978-9382956013).
- Kapoor, K. L., A Textbook of Physical Chemistry: States of Matter and Ions in Solution, Vol. I, 6th Ed., McGraw Hill Education India (2019). (ISBN: 978-9353165185).
- Bahl, A.; Bahl, B. S.; Tuli, G. D., Essentials of Physical Chemistry, 28th Ed., S. Chand and Company (2020). (ISBN: 978-9352836093)

## Semester III

|                              |                                                                   |
|------------------------------|-------------------------------------------------------------------|
| <i>NCrF level</i>            | 5.0                                                               |
| <i>Title of the Course</i>   | Core Chemistry- III                                               |
| <i>Course code</i>           | CHMM-301                                                          |
| <i>Paper credit</i>          | 04 ((L 4 – T 0 - P 0)                                             |
| <i>Total Contact Hours</i>   | Theory 70                                                         |
| <i>Distribution of Marks</i> | Theory 100 (End semester examination 70 + internal assessment 30) |

### Course Objectives

Upon successful completion of this course, students will be able to:

- Develop a comprehensive understanding of acid–base theories, aqueous acid–base equilibria, buffer systems, and factors governing the strength of acids and bases.
- Explain the principles of redox chemistry, electrochemical potentials, and their applications in redox reactions, electrochemical processes, and analytical chemistry.
- Understand the fundamental principles of extractive metallurgy and relate thermodynamic concepts to the extraction, purification, and refining of metals.
- Interpret the mechanisms, regioselectivity, stereoselectivity, and synthetic applications of addition and substitution reactions involving alkenes, alkynes, and aromatic compounds.
- Apply the laws of thermodynamics and thermochemistry to analyse energy changes, spontaneity, and equilibrium in physical and chemical processes.
- Understand the thermodynamic basis of chemical equilibrium and predict the effects of changes in temperature, pressure, and concentration on equilibrium systems.
- Develop competency in statistical analysis of experimental data, including estimation of errors, accuracy, precision, and confidence limits, for reliable interpretation of chemical measurements.
- Integrate concepts from inorganic, organic, analytical, and physical chemistry to solve qualitative and quantitative chemical problems using scientific reasoning.

### Course Outcomes (COs)

After successful completion of this course, the students will be able to:

- CO1: Explain various acid–base theories, calculate pH and buffer composition, interpret acid–base equilibria, and correlate molecular structure with the strength of organic and inorganic acids and bases.
- CO2: Analyse oxidation–reduction reactions using electrochemical principles, balance redox equations, apply the Nernst equation, interpret electrochemical diagrams (Latimer and Frost), and evaluate the feasibility of redox processes and titrations.
- CO3: Explain the thermodynamic and electrochemical principles involved in metallurgy, including ore processing, metal extraction, refining techniques, and the application of Ellingham diagrams.
- CO4: Analyse the mechanisms, regioselectivity, stereoselectivity, and synthetic applications of addition reactions of alkenes and alkynes, and electrophilic and nucleophilic aromatic substitution reactions.

- CO5: Apply the First Law of Thermodynamics, thermochemical principles, and energy relationships to calculate thermodynamic quantities, interpret energy changes, and analyse reversible and irreversible processes.
- CO6: Interpret chemical equilibrium using thermodynamic concepts, derive relationships among equilibrium constants, and predict the influence of external variables on equilibrium using Gibbs free energy and Le Chatelier's principle
- CO7: Apply statistical methods to evaluate experimental data by estimating errors, determining accuracy and precision, analysing confidence limits, and interpreting the reliability of analytical results.
- CO8: Integrate concepts from acid–base chemistry, redox chemistry, metallurgy, organic reaction mechanisms, thermodynamics, chemical equilibrium, and statistical analysis to solve multidisciplinary chemical problems and interpret experimental observations using scientific reasoning.

### **Unit I: Acid-base Chemistry I**

**Lecture/Marks: 07**

Acid-base concepts (various theories and application to different molecules), Measure of acid and base strength, gas phase proton affinity, Acid-base equilibria in aqueous solution (Proton transfer equilibria in water), pH, buffer, acid-base neutralisation curves; indicator, choice of indicators

The definition of pKa, organic acids and bases (factors affecting relative strength), substituents affect the pKa (carbon acid)

### **Unit II Redox reactions**

**Lecture/Marks:10**

Ion-electron method of balancing equation of redox reaction, Elementary idea on standard redox potentials with sign conventions, Redox half-reactions, standard potentials and spontaneity, trends in standard potentials, the electrochemical series, Nernst equation, (without derivation).Influence of complex formation, precipitation and change of pH on redox potentials,

Redox stability, Reaction with water, oxidation by atmospheric oxygen, disproportionation and comproportionation, relation between solubility and standard potential, Diagrammatic representation of potential data (Latimer diagram, Frost diagram of common elements)

Feasibility of a redox titration, redox potential at the equivalence point, redox indicators

### **Unit III Metallurgy**

**Lecture/Marks: 08**

Chief modes of occurrence of metals based on standard electrode potentials, concentration of ores, conversion of concentrated ore into metallic oxide, reduction of metal oxide, Ellingham diagrams for reduction of metal oxides and application, electrochemical principles of metallurgy, Electrolytic Reduction, Refining of metals (various methods like Electrolytic Kroll process, Parting process, van Arkel-de Boer process and Mond's process, Zone refining)

### **Unit IV: Stereochemistry – II**

**Lectures/Marks 10**

Chirality arising out of stereoaxis: stereoisomerism of substituted cumulenes with even and odd number of double bonds; chiral axis in allenes, spiro compounds, alkylidene cycloalkanes and biphenyls; related configurational descriptors (R<sub>a</sub>/S<sub>a</sub>); atropisomerism; racemization of chiral biphenyls.

Concept of prostereoisomerism: prostereogenic centre; concept of (pro)n-chirality: topicity of ligands and faces (elementary idea); pro-R/pro-S, pro-E/pro-Z and Re/Si descriptors; pro-R and pro-S descriptors of ligands on propseudoasymmetric centre.

### **Unit V: Organic Reaction of alkene and alkyne**

**Lecture/Marks: 15**

*Addition to C=C:* mechanism (with evidence wherever applicable), reactivity, regioselectivity (Markownikoff and anti-Markownikoff additions) and stereoselectivity; reactions: hydrogenation, halogenation, hydrohalogenation, hydration, oxymercuration demercuration, hydroboration-oxidation, epoxidation, syn and anti-hydroxylation, ozonolysis, addition of singlet and triplet carbenes; Simmons-Smith cyclopropanation reaction; electrophilic addition to diene (conjugated dienes and allene); radical addition: HBr addition; mechanism of allylic and benzylic bromination in competition with brominations across C=C; use of NBS; Birch reduction of benzenoid aromatics; interconversion of E- and Z- alkenes; contra-thermodynamic isomerization of internal alkenes.

*Addition to C≡C (in comparison to C=C):* mechanism, reactivity, regioselectivity (Markownikoff and anti-Markownikoff addition) and stereoselectivity; reactions: hydrogenation, halogenations, hydrohalogenation, hydration, oxymercuration demercuration, hydroboration-oxidation, dissolving metal reduction of alkynes (Birch); reactions of terminal alkynes by exploring its acidity; interconversion of terminal and non-terminal alkynes.

### **Unit VI: Thermodynamics I**

**Lecture/Marks: 10**

Basic Concept: open, closed and isolated systems and surroundings; Concept of work, heat and energy; Path function and State function, State of a system; Intensive and extensive variables Zeroth law of thermodynamics, 1st law of thermodynamics, concept of internal energy, enthalpy and heat capacity, mathematical proof of heat and work, change of energy and enthalpy function with temperature, relations between  $C_p$  and  $C_v$ , Joule-Thomson experiment, thermodynamic changes in isothermal and adiabatic change in volume of an ideal gas, comparison between reversible isothermal and adiabatic expansion of an ideal gas,

### **Unit I Chemical Kinetics I**

**Lecture Marks 10**

Brief overview of reaction rate, rate equation, order and molecularity Steady-state approximation and kinetics of simple reactions (e.g., decomposition of ozone, reaction between NO and  $O_2$ , iodination of acetone, decomposition of gaseous  $N_2O_5$ ).

Kinetics of complex reactions (integrated rate expressions up to first order only): (i) Opposing reactions (ii) parallel reactions, (iii) consecutive reactions.

#### **Suggested Readings**

- Lee, J. D. Concise Inorganic Chemistry, 5th Ed., Wiley India Pvt. Ltd., 2008.
- Atkin, P. Shriver & Atkins' Inorganic Chemistry, 5th Ed., Oxford University Press (2010).
- Atkins, P.W. & Paula, J. Physical Chemistry, Oxford Press, 2006.
- Winter, M. J., The Orbitron, <http://winter.group.shef.ac.uk/orbitron/> (2002). An illustrated gallery of atomic and molecular orbitals.
- Bruice, P. Y. (2016). *Organic Chemistry* (8th ed.). Pearson.
- March, J., Smith, M. B. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6th Edn., (Wiley, 2007).



## Semester III

|                              |                                                                             |
|------------------------------|-----------------------------------------------------------------------------|
| <i>NCrF level</i>            | 5.0                                                                         |
| <i>Title of the Course</i>   | <i>Core Chemistry- IV (Practical)</i>                                       |
| <i>Course code</i>           | <i>CHMM-302 (P)</i>                                                         |
| <i>Paper credit</i>          | <i>04 ((L 0 – T 0 - P 4)</i>                                                |
| <i>Total Contact Hours</i>   | <i>Practical 120</i>                                                        |
| <i>Distribution of Marks</i> | <i>Practical 100 (End semester examination 70 + internal assessment 30)</i> |

### Course Objectives

Upon successful completion of this laboratory course, students will be able to:

- Develop proficiency in classical laboratory techniques for the separation, purification, preparation, characterization, and qualitative analysis of organic and inorganic compounds.
- Acquire practical skills in volumetric analysis, inorganic synthesis, and analytical methods used for the identification and estimation of chemical substances.
- Understand the principles of physical chemistry through experiments involving surface tension, viscosity, thermochemistry, and related physicochemical measurements.
- Gain introductory knowledge of computational chemistry by employing molecular modelling software for molecular visualization, geometry optimization, and interpretation of molecular properties.
- Develop competence in recording observations, analysing experimental data, performing calculations, estimating experimental errors, and interpreting results using scientific principles.
- Foster safe laboratory practices, ethical conduct, teamwork, scientific communication, and proper handling and disposal of chemicals following green chemistry principles.

### Course Outcomes (COs)

After successful completion of this practical course, the students will be able to

CO1: Perform qualitative inorganic analysis to identify cations and anions,

CO2: Prepare coordination compounds and double salts, verify their composition, and distinguish between different classes of inorganic compounds using standard laboratory techniques.

CO3: Carry out volumetric analyses including acid–base, redox, and complexometric titrations to determine the concentration or composition of unknown samples with accuracy and precision.

CO4: Separate, purify, prepare, and characterize organic compounds using solvent extraction, crystallization, recrystallization, melting point determination

CO5: Perform qualitative organic analysis for the identification of functional groups and elements.

CO6: Use computational chemistry tools to construct molecular structures, perform geometry optimization, compare molecular properties, analyse molecular stability

CO7: Determine physicochemical properties such as surface tension, viscosity, enthalpy changes, heat capacity using appropriate experimental methods, graphical analysis, and calculations.

**Part A****i) Qualitative analysis of inorganic salt 20 hrs**

Analysis of a simple water soluble salt containing one or two cations and anions

*Marks distribution: Physical properties and solubility-01, Preliminary Dry tests for acid radicals-02, special confirmatory test for acid radicals – 02, Wet test for acid radicals-02, Group analysis -04 Conclusion and remarks-01, total =12 marks)*

**ii) Simple volumetric analysis 20 hrs**

Following estimations have to be performed

- Acid base titration: Estimation of carbonate, bicarbonate and hydroxide.
- Redox titration:
  - a) Estimation of oxalic acid by using standardised  $\text{KMnO}_4$  solution
  - b) Estimation of oxalic acid by  $\text{Fe(II)}$  using standardised  $\text{KMnO}_4$  solution
  - c) Determination of water of crystallisation of Mohr Salt using standardised  $\text{KMnO}_4$  solution
  - d) Estimation of  $\text{Fe(II)}$  with  $\text{K}_2\text{Cr}_2\text{O}_7$  using internal indicator
  - e) To determine the hardness of water by EDTA titration

**b) Inorganic Preparation 10 hrs**

Preparation of the following ( at least two compounds one from double salt and another from complex ions should be prepared and make them understand the difference between double salt and coordination complex):

- Mohr's salt
- Chrome alum
- Potash alum
- Tetramminecopper(II) sulphate
- $\text{Cu}(\text{glycinate})_2$
- Hexamminenickel(II) chloride
- Potassium trioxalato chromate(III)
- $[\text{Ni}(\text{DMG})_2]$

*Students should recrystallize the product and verify presence of anions and cations by qualitative analysis.*

*(Distribution of Marks: Experimentation–02, quality and quantity – 01+03=04, Result and conclusion – 2; total=08)*

**Part B****i) Separation of solid organic compound 10hrs**

Separation based upon solubility, by using common laboratory reagents like water (cold,hot), dil.  $\text{HCl}$ , dil.  $\text{NaOH}$ , dil.  $\text{NaHCO}_3$ , etc., of components of a binary solid mixture; purification of **any one** of the separated components by crystallization and determination of its melting point. The composition of the mixture should be of the following types **[minimum three]**:

- *p*-Nitrobenzoic acid/*p*-Aminobenzoic acid;
- *p*-Nitrotoluene/*p*-Anisidine;
- benzoic acid/naphthalene;

- urea/phenyl benzoate;
- *p*-toluidine/benzophenone;
- *p*-chlorobenzoic acid/ benzophenone,
- Benzoic acid/Anthracene;
- Glucose/Biphenyl;
- Benzoic acid/Benzophenone;
- Urea/Benzophenone.

Use of pH paper is recommended.

(Distribution of Marks: solubility separation-02, crystallization and quality =05, Result and conclusion – 03; total=10)

## ii) Preparation of organic compound and purification by recrystallization 10hrs

The following reactions are to be performed, noting the yield of the crude product: (student must perform at least three experiments)

- Cannizaro reaction of benzaldehyde (separation of benzyl alcohol and benzoic acid by solvent extraction)
- Reduction of benzophenone to benzhydrol
- Nitration of salicylic acid with ceric ammonium nitrate under greener method.
- Diazo-coupling reaction

Students must also calculate percentage yield, based upon isolated yield (crude) and theoretical yield. Purification of the crude product is to be made by crystallisation from water/alcohol, Crystallization after charcoal treatment, or sublimation, whichever is applicable. Melting point of the purified product is to be noted.

(Distribution of Marks: Experimentation –03, quality and quantity – 02+03=05, Result and conclusion – 2; total=10)

## iii) Qualitative analysis of an organic compound 20 hrs

- Detection of N, S, Halogens
- Test for functional groups

(Distribution of Marks: Detection of elements –02, Test for functional group – 04, solubility, aromaticity, unsaturation test, mp/bp – 02, Result and conclusion – 2; total=12)

## Part C

- i) Basic computational chemistry 10 hrs
- Familiarization with Avogadro/Jmol/IQmol/ORCA interface
  - Drawing and editing molecular structures
  - Geometry optimization of small molecules
  - Comparison of bond lengths in benzene and cyclohexane
  - Effect of substituents on dipole moment
  - Stability comparison of cis and trans isomers.

- Evaluating the compressibility factor using standard packages such as Excel/Origin/Python/Fortran.
- ii) Surface tension and viscosity 20 hrs
- Determine the surface tension of a given liquid at room temperature using stalagmometer by drop number method
  - Determine the surface tension of a given liquid by means of stalagmometer using drop weight method
  - Determine the composition of a given mixture by surface tension method.
  - Study the variation of surface tension of detergent solutions with concentration
  - Determine the viscosity of a liquid at a given concentration at laboratory temperature, by viscometer
  - Determine the composition of a given liquid mixture by viscosity method
  - Study the variation of viscosity of sucrose solution with the concentration of the solute
- iii) Thermochemistry 10 hrs
- Determination of heat capacity of a calorimeter and enthalpy of neutralisation (eg. hydrochloric acid with sodium hydroxide)
  - Determine the enthalpy of solution of oxalic acid from solubility measurements
  - Determination of heat capacity of a calorimeter for different volumes using change of enthalpy data of a known system (method of back calculation of heat capacity of calorimeter from known enthalpy of solution or enthalpy of neutralization)
  - Calculation of ionization enthalpy of ethanoic acid
  - Determination of enthalpy of hydration of copper sulphate.

(Distribution of Marks: Writing theory: 03, experimentation –02, Graphical representation of data/ tabulation - 03, Result and conclusion – 2; total=10)

Total marks: 70 (end semester examination) + 30 (internal)

Marks distribution: Part A: Inorganic (any two) experiment: 20, Part B: Organic (any two) experiment(s): 20, Part C: Physical (any two) experiment(s): 20, Viva: 10

### Suggested readings

- Vogel, A. I., Furniss, B. S., Hannaford, A. J., Smith, P. W. G., & Tatchell, A. R. *Vogel's Textbook of Practical Organic Chemistry*, 5th Edition, Pearson/Longman.
- Mendham, J., Denney, R. C., Barnes, J. D., & Thomas, M. J. K. *Vogel's Quantitative Chemical Analysis*, 6th Edition, Pearson Education.
- Svehla, G. *Vogel's Qualitative Inorganic Analysis*, 7th Edition, Pearson Education.
- Garland, C. W., Nibler, J. W., & Shoemaker, D. P. *Experiments in Physical Chemistry*, 8th Edition, McGraw-Hill.
- Khosla, B. D., Garg, V. C., & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Company.
- Ahluwalia, V. K., Dhingra, S., & Gulati, A. *College Practical Chemistry*, Universities Press.
- Mukherjee, B. K. *College Practical Chemistry*, New Central Book Agency.

## Semester IV

|                       |                                                            |
|-----------------------|------------------------------------------------------------|
| NCrF level            | 5.0                                                        |
| Title of the Course   | Inorganic Chemistry- I                                     |
| Course code           | CHMM-401                                                   |
| Paper credit          | 04 (L 4 – T 0 - P 0)                                       |
| Total Contact Hours   | Theory 70 hours                                            |
| Distribution of Marks | 100 (End semester examination 70 + internal assessment 30) |

### Course Objectives

The course is designed to

- To introduce the concepts of molecular symmetry and their applications in understanding the structure and properties of inorganic molecules and coordination compounds.
- To develop a comprehensive understanding of the chemistry of s-block and d-block elements, including their periodic trends, compounds and chemical behaviour.
- To explain the fundamental theories of bonding in coordination compounds and correlate their structures with magnetic and spectroscopic properties.
- To familiarize students with the biological significance of metal ions and their role in essential biochemical processes.
- To provide knowledge of important inorganic materials such as glass, ceramics, cements and alloys, emphasizing their preparation, properties and industrial applications.

### Course Outcomes (COs)

Upon successful completion of this course, students will be able to:

- CO1:** Explain molecular symmetry, identify symmetry elements and operations, assign point groups to simple molecules and coordination compounds, and relate symmetry to molecular structure.
- CO2:** Describe the chemistry of s-block and d-block elements, including their electronic configurations, oxidation states, periodic trends, preparation, properties and applications of their important compounds.
- CO3:** Apply Valence Bond Theory and Crystal Field Theory to predict the geometry, magnetic behaviour, stability and crystal field stabilization energy of coordination compounds.
- CO4:** Explain the biological importance of essential and trace metal ions, describe the transport and storage of metal ions in living systems, and discuss the structure and functions of important metalloproteins.
- CO5:** Describe the preparation, properties and industrial applications of inorganic materials such as glasses, ceramics, cements and alloys, and relate their composition to their physical and chemical properties.

### Unit I Introduction to molecular symmetry

**Lecture/Marks: 10**

Symmetry elements and operations, molecular point groups, symmetry elements present in  $C_{2v}$ ,  $C_{3v}$ ,  $D_{4h}$ ,  $T_d$  and  $O_h$  point groups (pictorial representation), Symmetry of octahedron, tetrahedron and square planar complexes, Structure and symmetry of inorganic compounds(coordination 2-8), Shape and symmetry of s, p and d orbitals,

Introductory idea of character tables, Mulliken symbols

**Unit II Main group elements I: s- block chemistry**

**Lecture/Marks: 15**

Relative stability of different oxidation states, diagonal relationship and anomalous behaviour of first member of each group, Complex formation tendency of s-elements.

- Hydrides and their classification: ionic, covalent and interstitial; basic beryllium acetate and nitrate
- Preparation and properties of oxides, superoxides, peroxides, hydrides, hydroxides, halides and carbonates of alkali and alkaline earth metals. Reactions of alkali and alkaline earth metals with oxygen, hydrogen, water and liquid ammonia
- Preparation and properties of Ortho and Para hydrogen

**Unit III d-block Chemistry**

**Lecture/Marks:10**

General periodic trends in d-block elements, chemistry of various oxidation states of transition metals, heavier transition elements, oxidation states and emf of groups 3-12, Halides and oxides of first row transition elements (Ti-Cu), Comparison of the first, second and third transition series elements

**Unit IV Coordination Chemistry II: Bonding Theories**

**Lecture/Marks:10**

Valence bond theory, inner and outer orbital complexes, electroneutrality principle and back bonding, effects of hybridization in metal-ligand bond strength and stability of complexes, choice of metal d-orbital(s) in hybridization in different coordination geometries, magnetic properties of complexes, drawback of VBT

Crystal Field Theory (qualitative treatment): d-orbital splitting in tetrahedral, and octahedral geometries, Calculation of CFSE, Thermodynamic and structural aspect of orbital splitting, pairing energies (contribution of exchange and coulomb energy), factors affecting the magnitude of  $10 Dq$  ( $\Delta_o$ ,  $\Delta_t$ ), spectrochemical series, merits and demerits of CFT.

**Unit V Bioinorganic Chemistry I**

**Lecture/Marks:10**

Essential and trace elements and their biological role, Effect of deficiency of some metal ions, Toxic effect of metal ions (Fe, Cu, Hg, Pb, Cd and As)

Importance of Na/K salts, calcium in biology, active transport of ions (Sodium -potassium pump)

Uptake, transport and storage of iron (ferritin, transferrin and siderophores), Introduction to the structure and function of haemoglobin

**Unit VI Inorganic materials of industrial importance**

**Lecture/Marks: 15**

Glass: Glassy state and its properties, classification (silicate and non-silicate glasses), manufacture and processing of glass, Composition and properties of the following types of glasses: Soda lime glass, lead glass, armoured glass, safety glass, borosilicate glass, fluorosilicate, coloured glass, photosensitive glass

Ceramics: Important clays and feldspar, ceramic, their types and manufacture, high technology ceramics and their applications, superconducting and semiconducting oxides

Cements: Classification of cement, ingredients and their role, Manufacture of cement and the setting process, quick setting cements.

Alloys: Classification of alloys, ferrous and nonferrous alloys, specific properties of elements in alloys. Manufacture of Steel (removal of silicon, decarbonization, demanganization, desulphurization, dephosphorisation), composition and properties of different types of steels.

*Suggested reading*

- Housecroft, C. E., & Sharpe, A. G. (2018). *Inorganic Chemistry* (5th ed.). Pearson Education Limited.
- Miessler, G. L., Fischer, P. J., & Tarr, D. A. (2014). *Inorganic Chemistry* (5th ed.). Pearson Education.
- Huheey, J. E., Keiter, E. A., Keiter, R. L., & Medhi, O. K. (2006). *Inorganic Chemistry: Principles of Structure and Reactivity* (4th Indian Reprint). Pearson Education.
- Cotton, F. A., Wilkinson, G., Murillo, C. A., & Bochmann, M. (1999). *Advanced Inorganic Chemistry* (6th ed.). Wiley.
- Shriver, D. F., Weller, M. T., Overton, T. L., Rourke, J. P., & Armstrong, F. A. (2014). *Shriver and Atkins' Inorganic Chemistry* (6th ed.). Oxford University Press.
- Lee, J. D. (2010). *Concise Inorganic Chemistry* (5th ed.). Wiley India.
- Malik, W. U., Tuli, G. D., & Madan, R. D. (Latest Edition). *Selected Topics in Inorganic Chemistry*. S. Chand Publishing.
- Greenwood, N. N., & Earnshaw, A. (1997). *Chemistry of the Elements* (2nd ed.). Butterworth-Heinemann.



## Semester IV

|                              |                                                            |
|------------------------------|------------------------------------------------------------|
| <i>NCrF level</i>            | 5.0                                                        |
| <i>Title of the Course</i>   | <i>Organic Chemistry - I</i>                               |
| <i>Course code</i>           | CHMM-402                                                   |
| <i>Paper credit</i>          | 04 (L 4 – T 0 - P 0)                                       |
| <i>Total Contact Hours</i>   | Theory 70 hours                                            |
| <i>Distribution of Marks</i> | 100 (End semester examination 70 + internal assessment 30) |

### Course Objectives

The course is designed to:

- To develop a comprehensive understanding of the mechanisms, selectivity and synthetic applications of aromatic substitution and carbonyl reactions.
- To explain the chemistry of carbonyl compounds, enolates,  $\alpha,\beta$ -unsaturated carbonyl systems and carboxylic acid derivatives, emphasizing reaction mechanisms and synthetic utility.
- To provide knowledge of the preparation, properties and reactions of nitrogen-containing organic compounds and their importance in organic synthesis.
- To introduce the fundamental principles and applications of solvent extraction and chromatographic techniques for the separation, purification and analysis of organic and inorganic compounds.
- To develop the ability to analyse organic reaction mechanisms and apply appropriate synthetic and separation strategies in solving chemical problems.

### Course Outcomes (COs)

Upon successful completion of the course, students will be able to:

- CO1:** Explain the mechanisms, orientation and reactivity of electrophilic and nucleophilic aromatic substitution reactions and predict the products of aromatic substitution reactions.
- CO2:** Interpret the chemistry of carbonyl compounds, including nucleophilic addition, substitution, condensation, oxidation, reduction and rearrangement reactions, and apply these transformations in multistep organic synthesis.
- CO3:** Describe the preparation, properties and reaction mechanisms of amines, nitro compounds, nitriles, isonitriles and diazonium salts, and evaluate their synthetic significance.
- CO4:** Apply the principles of solvent extraction and chromatographic techniques for the separation, purification and qualitative or quantitative analysis of chemical compounds.
- CO5:** Analyse reaction pathways, compare competing reaction mechanisms and design suitable synthetic routes using appropriate reagents and reaction conditions.

### Unit I: Organic Reactions: Aromatic substitution

**Lecture/Marks: 10**

*Aromatic Substitution Electrophilic aromatic substitution:* mechanisms and evidences in favour of it; orientation and reactivity; reactions: nitration, nitrosation, sulfonation, halogenation, Friedel-Crafts reaction; one-carbon electrophiles (reactions: chloromethylation, 25 Gatterman-Koch, Gatterman, Houben-Hoesch, Vilsmeier-Haack, Reimer-Tiemann, Kolbe-Schmitt); Ipso substitution.

*Nucleophilic aromatic substitution:* addition-elimination mechanism and evidences in favour of it; SN1 mechanism; cine substitution (benzyne mechanism), structure of benzyne

**Unit-II: Carbonyl and Related Compounds****Lecture/Marks: 30**

Addition to C=O: structure, reactivity and preparation of carbonyl compounds; mechanism (with evidence), reactivity, equilibrium and kinetic control; formation of hydrates, cyanohydrins and bisulphite adduct; nucleophilic addition-elimination reactions with alcohols, thiols and nitrogen-based nucleophiles; reactions: benzoin condensation, Cannizzaro and Tischenko reactions, reactions with ylides: Wittig and Corey-Chaykovsky reaction; Rupe rearrangement, oxidations and reductions: Clemmensen, Wolff-Kishner,  $\text{LiAlH}_4$ ,  $\text{NaBH}_4$ , MPV, Oppenauer, Bouveault-Blanc, acyloin condensation; oxidation of alcohols with PDC and PCC; periodic acid and lead tetraacetate oxidation of 1,2-diols.

Exploitation of acidity of  $\alpha$ -H of C=O: formation of enols and enolates; kinetic and thermodynamic enolates; reactions (mechanism with evidence): halogenation of carbonyl compounds under acidic and basic conditions, Hell-Volhard-Zelinsky (H. V. Z.) reaction, nitrosation,  $\text{SeO}_2$  (Riley) oxidation; condensations (mechanism with evidence): Aldol, Tollens', Knoevenagel, Claisen-Schmidt, Claisen ester including Dieckmann, Stobbe; Mannich reaction, Perkin reaction, Favorskii rearrangement; alkylation of active methylene compounds; preparation and synthetic applications of diethyl malonate and ethyl acetoacetate; specific enol equivalents (lithium enolates, enamines and silyl enol ethers) in connection with alkylation, acylation and aldol type reaction.

Nucleophilic addition to  $\alpha,\beta$ -unsaturated carbonyl system: general principle and mechanism (with evidence); direct and conjugate addition, addition of enolates (Michael reaction), Stetter reaction, Robinson annulation.

Substitution at  $\text{sp}^2$  carbon (C=O system): mechanism (with evidence):  $B_{\text{AC}2}$ ,  $A_{\text{AC}2}$ ,  $A_{\text{AC}1}$ ,  $A_{\text{AL}1}$  (in connection to acid and ester); acid derivatives: amides, anhydrides & acyl halides (formation and hydrolysis including comparison).

**Unit III: Carboxylic Acids and their Derivatives****Lecture Marks: 15**

Preparation, physical properties and reactions of monocarboxylic acids. Typical reactions of dicarboxylic acids, hydroxy acids and unsaturated acids: succinic/phthalic, lactic, malic, tartaric, citric, maleic and fumaric acids. Preparation and reactions of sulphonic acids.

Preparation and reactions of acid chlorides, anhydrides, esters and amides; Mechanism of acidic and alkaline hydrolysis of esters, Claisen condensation, Dieckmann and Reformatsky reactions, Hofmann bromamide degradation and Curtius rearrangement.

**Unit-IV: Separation techniques****Lecture/Marks: 15**

Solvent extraction: Classification, principle and efficiency of the technique, Mechanism of extraction, extraction by solvation and chelation, Technique of extraction: batch, continuous and counter current extractions, Qualitative and quantitative aspects of solvent extraction: extraction of metal ions from aqueous solution, extraction of organic species from the aqueous and nonaqueous media.

Chromatography: Classification, principle and efficiency of the technique, Mechanism of separation: adsorption, partition & ion exchange, Development of chromatograms: frontal, elution and displacement methods, Qualitative and quantitative aspects of chromatographic methods of analysis: IC, GLC, GPC, TLC and HPLC.

*Suggested readings*

- Clayden, J., Greeves, N., & Warren, S. (2021). *Organic Chemistry* (3<sup>rd</sup> ed.). Oxford University Press.
- Solomons, T. W. G., Fryhle, C. B., & Snyder, S. A. (2023). *Organic Chemistry* (13<sup>th</sup> ed.). John Wiley & Sons.
- Bruice, P. Y. (2016). *Organic Chemistry* (8<sup>th</sup> ed.). Pearson Education.
- Carey, F. A., & Giuliano, R. M. (2022). *Organic Chemistry* (11<sup>th</sup> ed.). McGraw-Hill Education.
- Carey, F. A., & Sundberg, R. J. (2007). *Advanced Organic Chemistry, Part B: Reactions and Synthesis* (5<sup>th</sup> ed.). Springer.
- Smith, M. B. (2020). *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure* (8<sup>th</sup> ed.). Wiley.
- Norman, R. O. C., & Coxon, J. M. (1993). *Principles of Organic Synthesis* (3<sup>rd</sup> ed.). Chapman & Hall.
- Caruthers, W., & Coldham, I. (2004). *Modern Methods of Organic Synthesis* (4<sup>th</sup> ed.). Cambridge University Press.
- Harwood, L. M., Moody, C. J., & Percy, J. M. (2017). *Experimental Organic Chemistry: Principles and Practice* (2<sup>nd</sup> ed.). Wiley-Blackwell.
- Skoog, D. A., Holler, F. J., & Crouch, S. R. (2018). *Principles of Instrumental Analysis* (7<sup>th</sup> ed.). Cengage Learning.

## Semester IV

|                              |                                                            |
|------------------------------|------------------------------------------------------------|
| <i>NCrF level</i>            | 5.0                                                        |
| <i>Title of the Course</i>   | <i>Physical Chemistry - I</i>                              |
| <i>Course code</i>           | CHMM-403                                                   |
| <i>Paper credit</i>          | 04 (L 4 – T 0 - P 0)                                       |
| <i>Total Contact Hours</i>   | Theory 70 hours                                            |
| <i>Distribution of Marks</i> | 100 (End semester examination 70 + internal assessment 30) |

### Course Objectives

The course is designed to

- To develop a fundamental understanding of thermodynamic principles governing chemical reactions and energy changes.
- To explain the behaviour of ideal and non-ideal solutions, phase equilibria, colloidal systems and ionic equilibria through thermodynamic and physicochemical concepts.
- To provide knowledge of acid-base equilibria, buffer systems, solubility equilibria and their applications in analytical, biological and industrial chemistry.
- To introduce the fundamental principles of quantum mechanics and demonstrate their application to simple microscopic systems.
- To develop the ability to apply physical chemistry concepts and mathematical reasoning to solve quantitative chemical problems and interpret physicochemical phenomena.

### Course Outcomes (COs)

Upon successful completion of the course, students will be able to:

- CO1:** Explain thermochemical concepts, calculate various thermodynamic quantities using Hess's law and Kirchhoff's equations, and interpret the energetics of chemical reactions.
- CO2:** Describe the properties of ideal and non-ideal solutions, phase behaviour, distribution equilibria and solvent extraction, and apply these concepts to chemical systems.
- CO3:** Explain the preparation, properties, stability and applications of colloidal systems and relate colloidal phenomena to industrial and biological processes.
- CO4:** Apply the principles of ionic equilibrium to calculate pH, buffer capacity, hydrolysis, solubility products and acid-base titration behaviour in aqueous systems.
- CO5:** Explain the postulates of quantum mechanics, solve simple quantum mechanical problems such as the particle-in-a-box model, and interpret the quantum behaviour of microscopic systems.

### Unit I Thermodynamic-II

**Lecture Marks 10**

Thermochemistry: Heats of reactions, enthalpy of formation of molecules and ions and enthalpy of combustion; Enthalpy of reaction; Hess's law, various types of enthalpies, of reactions, calculation of bond energy, bond dissociation energy and resonance energy from thermochemical data, effect of temperature (Kirchhoff's equations) and pressure on enthalpy of reactions. Adiabatic flame temperature, explosion temperature

**Unit II Solutions****Lecture Marks 15**

Types of solutions, concentration units, Solution of gases in liquids-Henry's law. Solution of liquids in liquids: Thermodynamics of ideal solutions: Ideal solutions and Raoult's law, deviations from Raoult's law –non-ideal solutions. Vapour pressure-composition and temperature composition curves of ideal and non-ideal solutions. Distillation of solutions. Lever rule, Azeotropes. Partial miscibility of liquids: Critical solution temperature; effect of impurity on partial miscibility of liquids. Immiscibility of liquids-Principle of steam distillation. Nernst distribution law and its applications, solvent extraction. Solutions of solids in liquids: the solubility curves.

**Unit III Colloids****Lecture Marks 10**

Classification of colloids; preparation of colloids- peptisation, Bredig's method and condensation methods; purification of colloids, properties of colloids- Tyndall effect-Brownian movement, electrophoresis and electro-osmosis, electrical double layer and zeta potential, theory of stabilities of colloids, protective action of Lyophilic sol, gold number, determination of Avogadro's number, coagulation of colloids, Schultz-Hardy rule, association of colloids, emulsions, micelles and their structure, critical micelles concentration, Donnan membrane equilibria

**Unit VI Chemical Equilibrium****Lecture/Marks: 15**

Criteria of thermodynamic equilibrium, degree of advancement of reaction, chemical equilibria in ideal gases, concept of fugacity, Thermodynamic derivation of relation between Gibbs free energy of reaction and reaction quotient, Coupling of exoergic and endoergic reactions, Equilibrium constants and their quantitative dependence on temperature, pressure and concentration, Free energy of mixing and spontaneity; thermodynamic derivation of relations between the various equilibrium constants  $K_p$ ,  $K_c$  and  $K_x$ . Le Chatelier's principle (quantitative treatment); equilibrium between ideal gases and a pure condensed phase.

**Unit IV Quantum Mechanics-I****Lecture Marks 20**

A brief review of the failure of classical mechanics (Planck's quantum theory, photoelectric effect, wave-particle duality, uncertainty principle)

Time-independent Schrödinger equation and properties of wave functions, Postulates of quantum mechanics; normalization and orthogonality; quantum mechanical operators; properties of operators; eigenvalues and eigenfunctions; setting up of operators for different observables; orbital angular momentum operators; Hermitian operators; Schmidt-orthogonalization technique.

Particle in a one-dimensional box; characteristics of wave functions; quantization of energy levels; zero-point energy and Heisenberg uncertainty principle; probability distribution functions and nodal properties.

Three-dimensional box; separation of variables; degree of degeneracy; concept of tunnelling.

**Suggested Readings**

- Atkins, P., de Paula, J., & Keeler, J. (2023). *Atkins' Physical Chemistry* (12th ed.). Oxford University Press.
- Engel, T., & Reid, P. (2019). *Physical Chemistry* (4th ed.). Pearson Education.
- Castellan, G. W. (1983). *Physical Chemistry* (3rd ed.). Narosa Publishing House.

- Levine, I. N. (2014). *Physical Chemistry* (6th ed.). McGraw-Hill Education.
- McQuarrie, D. A., & Simon, J. D. (1997). *Physical Chemistry: A Molecular Approach*. University Science Books.
- Mortimer, R. G. (2008). *Physical Chemistry* (3rd ed.). Elsevier Academic Press.
- Barrow, G. M. (1996). *Physical Chemistry* (6th ed.). Tata McGraw-Hill.
- Glasstone, S. (2007 Reprint). *Textbook of Physical Chemistry*. Macmillan India Ltd.
- Maron, S. H., & Prutton, C. F. (2006 Reprint). *Principles of Physical Chemistry*. Oxford & IBH Publishing.
- Puri, B. R., Sharma, L. R., & Pathania, M. S. (Latest Edition). *Principles of Physical Chemistry*. Vishal Publishing Co.
- Sen, B. K., *Quantum Chemistry including Spectroscopy*, 4th edition, Kalyani Publishers
- Bhattacharyya, P.K., *Fundamentals of Quantum Chemistry*, Global Publishing House (India)

## Semester IV

|                              |                                                                   |
|------------------------------|-------------------------------------------------------------------|
| <i>NCrF level</i>            | 5.0                                                               |
| <i>Title of the Course</i>   | <i>Organic Chemistry Practical- I</i>                             |
| <i>Course code</i>           | <i>CHMM-404(P)</i>                                                |
| <i>Paper credit</i>          | <i>04 (L 0 – T 0 - P 4)</i>                                       |
| <i>Total Contact Hours</i>   | <i>Practical 120 hours</i>                                        |
| <i>Distribution of Marks</i> | <i>100 (End semester examination 70 + internal assessment 30)</i> |

### Course Objectives

The course is designed to:

- To develop practical skills in the synthesis, purification and characterization of organic compounds using conventional and green chemistry approaches.
- To familiarize students with chromatographic techniques for the separation, identification and purification of organic compounds.
- To impart quantitative analytical skills for the estimation of biologically and industrially important compounds using classical analytical methods.
- To provide hands-on training in the extraction and isolation of naturally occurring organic compounds using conventional and environmentally benign methods.
- To develop competence in laboratory safety, scientific observation, data recording, result interpretation and preparation of laboratory reports.

### Course Outcomes (COs)

Upon successful completion of this course, students will be able to:

- CO1:** Perform the synthesis of selected organic compounds using conventional and green chemistry methods, and evaluate reaction efficiency through purification and yield calculations.
- CO2:** Apply paper chromatography and thin-layer chromatography (TLC) for the separation, identification and analysis of organic compounds.
- CO3:** Carry out quantitative estimations of biomolecules and physicochemical parameters such as glucose, glycine, iodine value and saponification value with accuracy and precision.
- CO4:** Isolate and extract naturally occurring organic compounds using suitable extraction techniques and explain the principles underlying these methods.
- CO5:** Demonstrate good laboratory practices, maintain experimental records, analyse experimental data, and interpret results while adhering to laboratory safety and ethical standards.

### UNIT I: Organic Preparations

**Laboratory hours: 30; marks:15**

- Benzoylation of organic compounds: amines (aniline, toluidines, anisidine) and phenols (phenol,  $\beta$ -naphthol, salicylic acid) by both conventional method and green chemical approach. (atleast two from each)
- Bromination of acetanilide by conventional methods (ii) Nitration of salicylic acid using ceric ammonium (green chemistry approach) (iii) Selective reduction of *m*-dinitrobenzene to *m*-nitroaniline (iv) Oxidation of ethanol/isopropanol (iodoform reaction) (v) Aldol condensation using either conventional or green method, (vi) Benzil–Benzilic acid rearrangement.

### UNIT II: Chromatographic separation

**Laboratory hours: 30 marks: 15**



- Separation of a mixture of two amino acids by ascending paper chromatography
- Separation of a mixture of *o*- and *p*-nitrophenol or *o*- and *p*-nitroaniline by thin layer chromatography (TLC).

**UNIT III: Quantitative analysis**

**Laboratory hours: 25 /marks: 30**

- Estimation of Glucose
- Estimation of glycine by Sorenson's formalin method.
- Study of the titration curve of glycine (by pH metric methods).
- Determination of Iodine number of vegetable oil or a fat.
- Saponification value of vegetable oil or a fat.

**UNIT IV: Extraction**

**Laboratory hours: 30 /marks: 15**

- Extraction of D-limonene from orange peel by the conventional method/ using liquid CO<sub>2</sub> prepared from dry ice
- Extraction of caffeine from commercially available tea leaves
- Photoreduction of benzophenone to benzopinacol in the presence of sunlight/UV irradiation

**Suggested readings**

- Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A. J. and Smith, P.W.G., Textbook of Practical Organic Chemistry, 5thEdn., (Prentice-Hall, 1996).
- Mann, F.G. and Saunders, B.C. Practical Organic Chemistry, (Orient-Longman, 1960).
- Furniss, B. S., Ford, A. J. H., Smith, P. W. H. and Tatchell, A. R. Vogel's Textbook of Practical Organic Chemistry, 5thEdn., (John Wiley, 1989).
- Vishnoi, R. Advanced Practical Organic Chemistry, 2nd Revised Edn. (Vikas Publisher, 2007).

## Semester V

|                              |                                                                   |
|------------------------------|-------------------------------------------------------------------|
| <i>NCrF level</i>            | 5.5                                                               |
| <i>Title of the Course</i>   | <i>Inorganic Chemistry - II</i>                                   |
| <i>Course code</i>           | <i>CHMM-501</i>                                                   |
| <i>Paper credit</i>          | <i>04 (L 4 – T 0 - P 0)</i>                                       |
| <i>Total Contact Hours</i>   | <i>Theory 70 hours</i>                                            |
| <i>Distribution of Marks</i> | <i>100 (End semester examination 70 + internal assessment 30)</i> |

### Course Objectives

The course is designed to

- To develop a comprehensive understanding of modern acid–base theories and their applications in predicting the behaviour and reactivity of inorganic compounds.
- To explain the chemistry of p-block elements with emphasis on structure, bonding, preparation, properties and applications of their important compounds.
- To introduce advanced concepts of coordination chemistry, including crystal field stabilization, Jahn–Teller distortion and molecular orbital approach to metal–ligand bonding.
- To provide knowledge of nuclear chemistry, radioactive processes, nuclear reactions and the applications of radioisotopes in science, medicine and industry.
- To familiarize students with the role of metal ions in biological systems and the structure and functions of biologically important metalloproteins and metal-based drugs.

### Course Outcomes (COs)

Upon successful completion of the course, students will be able to:

- CO1:** Explain advanced acid–base concepts including HSAB theory, solvent effects, superacids, superbases and predict the stability and reactivity of inorganic compounds using modern acid–base principles.
- CO2:** Describe the chemistry of p-block elements, including their oxidation states, structure, bonding, preparation, properties and applications of important compounds and noble gas chemistry.
- CO3:** Apply Crystal Field Theory and introductory Molecular Orbital Theory to explain the electronic structure, magnetic behaviour, stability and geometries of coordination compounds.
- CO4:** Explain the principles of nuclear chemistry, radioactive decay, nuclear reactions and radioisotope applications in medicine, industry, agriculture and analytical chemistry.
- CO5:** Interpret the structure–function relationships of metalloproteins and metalloenzymes, explain the biological roles of metal ions and discuss the therapeutic applications of metal-based drugs.

### Unit I Acid-base Chemistry II

**Lecture/Marks: 10**

Frontier orbitals and acid base reaction, hydrogen bonding and acidity and basicity, Acids and bases in water, levelling effect, acid strength of binary hydrogen compounds, inductive effect and strength of oxyacids, acidity of aqua ions, steric effect, proton sponge, solvation effect and acid base anomalies, acid base strength in non-aqueous solvents, superacids and superbases Hard and Soft Acids and Bases (HSAB), Application of HSAB principle, symbiosis, Pearson paradox

**Unit II Main group elements II: p-block elements****Lecture/Marks: 20**

Relative stability of different oxidation states, diagonal relationship and anomalous behaviour of first member of each group; Complex formation tendency of *p-block* elements; Allotropy and catenation

Study of the following compounds with emphasis on structure, bonding, preparation, properties and uses: borane (bonding in diborane), ammonia, phosphine and hydrogen sulphide oxides of nitrogen, phosphorus and sulphur; Oxyacid's of nitrogen, phosphorus, sulphur, and chlorine; halides of silicon and phosphorus; borazine, phosphazene, boric acid, borax,  $S_4N_4$ ; Interhalogen compounds, polyhalides, pseudo halogen; silanes

Occurrence and uses noble gases, rationalisation of inertness of noble gases, preparation and properties of  $XeF_2$ ,  $XeF_4$  and  $XeF_6$ , Nature of bonding in noble gas compounds (Valence bond treatment and MO treatment for  $XeF_2$ ), Molecular shapes of noble gas compounds using VSEPR theory.

**Unit III Coordination chemistry III:****Lecture/Marks: 10**

Consequences of CFSE, Jahn-Teller Theorem, d-orbital splitting in square planar, trigonal bipyramidal, and square pyramidal geometries, consequences of Jahn-Teller theorem, site selection in spinel and inverse spinel structures.

Evidences of metal-ligand covalent character, Introduction to Molecular orbital theory

**Unit V Nuclear Chemistry****Lecture/Marks: 15**

Composition of nucleus, Elementary Particles, Composite Particles, Mass defect and binding energy, nuclear stability, packing fractions, fundamentals of radioactive decay, nuclear models, nuclear reactions, nuclear Fusion and Fission, radioactive decay and equilibrium, nuclear reaction Q value, Nuclear cross sections, nuclear reactor and its components, measurement of radioactivity, radioactive disintegration, law of successive disintegration, artificial radioactivity, applications of radioactive isotopes in studying reaction mechanism, in diagnosis and treatment of diseases, in industry, in agriculture, in analytical chemistry, in determination of the age of the earth by rock dating method and determination of the age of recent objects by radio carbon dating method.

**Unit IV Bioinorganic Chemistry II****Lecture/Marks: 15**

Structure function relationship of haemoglobin and myoglobin (cooperativity and Bohr effect), poisoning effect of CO and other ligands, genetic defects, synthetic dioxygen carriers, dioxygen toxicity, active site structure and function of Hemocyanin, Hemerythrin

Active site structure and functions of Rubredoxin, Ferredoxin ( $Fe_2S_2$ ,  $Fe_4S_4$ ), Cytochrome P450, catalases and peroxidases

Metalloenzymes: carboxypeptidase, carbonic anhydrase and superoxide dismutase, and blue copper proteins

Metals in medicine, Chelate therapy, Cisplatin as anticancer drug

**Suggested readings**

- Miessler, G. L., Fischer, P. J., & Tarr, D. A. *Inorganic Chemistry* (5th ed.). Pearson.
- Lee, J. D. *Concise Inorganic Chemistry* (5th ed.). Wiley India.
- Huheey, J. E., Keiter, E. A., Keiter, R. L., & Medhi, O. K. *Inorganic Chemistry: Principles of Structure and Reactivity* (4th Indian Reprint). Pearson.
- Arnika, H. J. (2016). *Essentials of Nuclear Chemistry* (4th ed.). New Age International (P) Ltd.
- Bertini, I., Gray, H. B., Stiefel, E. I., & Valentine, J. S. *Biological Inorganic Chemistry: Structure and Reactivity*. University Science Books.

## Semester V

|                              |                                                                   |
|------------------------------|-------------------------------------------------------------------|
| <i>NCrF level</i>            | 5.5                                                               |
| <i>Title of the Course</i>   | <i>Organic Chemistry – II</i>                                     |
| <i>Course code</i>           | <i>CHMM-502</i>                                                   |
| <i>Paper credit</i>          | <i>04 (L 4 – T 0 - P 0)</i>                                       |
| <i>Total Contact Hours</i>   | <i>Theory 70 hours</i>                                            |
| <i>Distribution of Marks</i> | <i>100 (End semester examination 70 + internal assessment 30)</i> |

### Course Objectives

The course is designed to

- To develop a comprehensive understanding of molecular rearrangements and their mechanistic pathways, enabling students to predict reaction outcomes and design synthetic strategies.
- To provide in-depth knowledge of the chemistry of heterocyclic and polynuclear aromatic compounds, including their synthesis, reactivity, orientation, biological significance and applications in organic synthesis.
- To introduce modern organometallic reagents and transition metal-catalysed cross-coupling reactions that form the basis of contemporary organic synthesis.
- To impart a fundamental understanding of molecular spectroscopy, including rotational, vibrational, Raman and electronic spectroscopy, for the structural elucidation and characterization of organic molecules.
- To develop the ability to interpret reaction mechanisms and spectroscopic data, correlate molecular structure with physical properties, and apply these concepts in advanced organic synthesis, medicinal chemistry and chemical research.

### Course Outcomes (COs)

Upon successful completion of the course, students will be able to:

- CO1: Explain the mechanisms, stereochemical aspects and synthetic significance of molecular rearrangement reactions and predict the products of complex organic transformations.
- CO2: Describe the synthesis, structure, aromaticity, reactivity and biological importance of heterocyclic and polynuclear aromatic compounds, and apply retrosynthetic approaches for their preparation.
- CO3: Explain the principles and synthetic applications of organometallic reagents and transition metal-catalysed cross-coupling reactions in carbon–carbon and carbon–heteroatom bond formation.
- CO4: Interpret rotational, vibrational, Raman and electronic spectra of organic molecules, correlate spectral features with molecular structure, and identify functional groups using spectroscopic techniques.
- CO5: Integrate mechanistic reasoning with spectroscopic evidence to solve structural and synthetic problems in organic chemistry and evaluate reaction pathways for the synthesis of target molecules.

**Unit I: Alcohol and phenols****Lecture/Marks: 25**

Alcohols: preparation, properties and relative reactivity of 1°, 2°, 3° alcohols, Bouvaelt-Blanc reduction; preparation and properties of glycols: oxidation by periodic acid and lead tetraacetate, Pinacol-Pinacolone rearrangement.

Phenols: Preparation and properties; acidity and factors affecting it, ring substitution reactions, Reaction of phenols: Reimer- Tiemann reaction, Kolbe's reaction, Lederer-Manasse reaction, Fries rearrangement, Claisen rearrangement, nitration, sulphonation, halogenation, oxidation, coupling with diazonium salt, oxidation of phenols by hypervalent iodine(III) reagents and other oxidizing agents to quinones; Reactions of quinones: Reactions with HCl, amines, alcohols, Thiele acetylation and dienone phenol rearrangement.

Ethers and Epoxides: Preparation and reactions with acids. Dialkyl, aryl alkyl and diaryl ethers; cyclic ethers: epoxides, oxetanes, THF, THP. Synthesis: Williamson ether synthesis, dehydration of alcohols, alkoxy mercuriation-demercuration, diaryl- and aryl alkyl ethers by S<sub>N</sub>Ar, cycloetherification. Reactions: S<sub>N</sub>1/S<sub>N</sub>2 cleavage of ethers by HI, HBr, BBr<sub>3</sub>, TMSI, NaSR. Reactions of epoxides with alcohols, ammonia derivatives and LiAlH<sub>4</sub>

Preparation and reactions of thiols and thioethers

Preparation and properties of Glycol: Oxidation by OsO<sub>4</sub>, alkaline, KMnO<sub>4</sub>, periodic acid and lead tetraacetate. Pinacol Pinacolone rearrangement with mechanism, Trihydric alcohol: Glycerol: preparation & properties. Other aromatic Hydroxy compounds: Cresol, nitrophenols, picric acid, benzyl alcohol, dihydric phenols.

**Unit II Alkyl and Aryl halides****Lecture Marks 10**

Alkyl halides: Preparation from alkenes and alcohols, Reactions: Hydrolysis, nitrite and nitro formation, Williamson's Synthesis: elimination vs Substitution

Aryl halides: Preparation (chloro, bromo, iodo benzene only) from phenol, Sandmeyer & Gattermann reaction, Reactions (chlorobenzene): Aromatic nucleophilic substitution (replacement by -OH) and effect of nitro substituent. Reactivity and relative strength of carbon-halogen bond in alkyl, allyl, benzyl and vinyl and Aryl halide.

**Unit-III: Nitrogen and sulphur containing compounds****Lecture/Marks: 20**

Amines: Aliphatic & Aromatic: preparation, separation (Hinsberg's method) and identification of primary, secondary and tertiary amines; reaction (with mechanism): Eschweiler-Clarke methylation, diazo coupling reaction, formation and reactions of phenylenediamines, diazomethane and diazoacetic ester.

Nitro compounds (aliphatic and aromatic): preparation and reaction (with mechanism): reduction under different conditions; Nef carbonyl synthesis, Henry reaction and conjugate addition of nitroalkane anion.

Alkyl nitrile and isonitrile: preparation and reaction mechanism, Thorpe nitrile condensation, von Richter reaction.

Diazonium salts and their related compounds: reactions (with mechanism) involving replacement of diazo group; reactions: Gomberg, Meerwein, Japp-Klingermann.

Sulphur containing compounds: Preparation and reactions of thiols, thioethers and sulphonic acids.

### Carbohydrates

Lecture Marks 15

Occurrence, classification and their biological importance

Monosaccharides: Aldoses up to 6 carbons; structure of D-glucose & D-fructose (configuration & conformation); ring structure of monosaccharides (furanose and pyranose forms): Haworth representations and non-planar conformations; anomeric effect (including stereoelectronic explanation); mutarotation; epimerization; reactions (mechanisms in relevant cases): Fischer glycosidation, osazone formation, bromine water oxidation, HNO<sub>3</sub> oxidation, selective oxidation of terminal –CH<sub>2</sub>OH of aldoses, reduction to alditols, Lobry de Bruyn-van Ekenstein rearrangement; stepping-up (Kiliani-Fischer method) and stepping-down (Ruff's & Wohl's methods) of aldoses; end-group-interchange of aldoses; acetonide (isopropylidene and benzylidene protections; ring size determination; Fischer's proof of configuration of (+)-glucose. Disaccharides: Glycosidic linkages, concept of glycosidic bond formation by glycosyl donor-acceptor, structure of sucrose.

### Suggested readings

- Clayden, J., Greeves, N., & Warren, S. *Organic Chemistry* (3rd ed.). Oxford University Press, 2021.
- Solomons, T. W. G., Fryhle, C. B., & Snyder, S. A. *Organic Chemistry* (13th ed.). John Wiley & Sons, 2023.
- Bruice, P. Y. *Organic Chemistry* (8th ed.). Pearson Education, 2016.
- Smith, M. B. *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure* (8th ed.). Wiley, 2020.
- Carey, F. A., & Sundberg, R. J. *Advanced Organic Chemistry, Part B: Reactions and Synthesis* (5th ed.). Springer, 2007.
- Gilchrist, T. L. *Heterocyclic Chemistry* (4th ed.). Pearson Education, 2010.
- Silverstein, R. M., Webster, F. X., Kiemle, D. J., & Bryce, D. L. *Spectrometric Identification of Organic Compounds* (8th ed.). Wiley, 2015.
- Pavia, D. L., Lampman, G. M., Kriz, G. S., & Vyvyan, J. R. *Introduction to Spectroscopy* (5th ed.). Cengage Learning, 2015.
- Kemp, W. *Organic Spectroscopy* (3rd ed.). Macmillan Press, 1991.
- Banwell, C. N., & McCash, E. M. *Fundamentals of Molecular Spectroscopy* (4th ed.). McGraw-Hill Education, 1994.
- Caruthers, W., & Coldham, I. *Modern Methods of Organic Synthesis* (4th ed.). Cambridge University Press, 2004.

## Semester V

|                              |                                                                   |
|------------------------------|-------------------------------------------------------------------|
| <i>NCrF level</i>            | 5.5                                                               |
| <i>Title of the Course</i>   | <i>Physical Chemistry - II</i>                                    |
| <i>Course code</i>           | <i>CHMM-503</i>                                                   |
| <i>Paper credit</i>          | <i>04 (L 4 – T 0 - P 0)</i>                                       |
| <i>Total Contact Hours</i>   | <i>Theory 70 hours</i>                                            |
| <i>Distribution of Marks</i> | <i>100 (End semester examination 70 + internal assessment 30)</i> |

### Course Objectives

After successful completion of this course, students will be able to

- Develop a comprehensive understanding of the fundamental principles of chemical thermodynamics, ionic equilibrium, colligative properties, thermochemistry, and molecular spectroscopy.
- Explain the concepts of entropy, free energy, spontaneity, equilibrium, and their applications in physical and chemical processes.
- Apply thermodynamic principles to calculate energy changes, equilibrium parameters, colligative properties, and thermochemical quantities in chemical systems.
- Understand the behaviour of electrolytic solutions, acid-base equilibria, buffer systems, solubility equilibria, and their applications in analytical and biological systems.
- Acquire knowledge of molecular spectroscopy, including rotational, vibrational, Raman, and electronic spectroscopy, for structural characterization of molecules.
- Interpret spectroscopic data to identify molecular structures, functional groups, bonding characteristics, and electronic transitions.
- Develop analytical, quantitative, and problem-solving skills through the application of thermodynamic, equilibrium, and spectroscopic principles to real-world chemical problems.

### Course Outcomes (COs)

Upon successful completion of the course, students will be able to:

**CO1:** Explain the second law of thermodynamics, entropy, Gibbs and Helmholtz free energy functions, spontaneity criteria, Maxwell relations, Joule–Thomson effect, and heat capacity relationships in chemical systems.

**CO2:** Apply thermodynamic principles to evaluate entropy changes, free energy changes, equilibrium conditions, useful work, phase transitions, and energy transformations in physical and chemical processes.

**CO3:** Analyze ionic equilibria in aqueous solutions by calculating pH, ionization constants, hydrolysis constants, buffer capacities, solubility products, and interpreting acid-base titration behaviour.

**CO4:** Apply the principles of colligative properties and thermochemistry to determine molecular masses, associated and dissociated solutes, enthalpy changes, bond energies, and temperature effects on chemical reactions.



**CO5:** Explain the fundamental principles of molecular spectroscopy, including rotational, vibrational, Raman, and electronic spectroscopy, and their interaction with electromagnetic radiation.

**CO6:** Interpret infrared, Raman, UV–Visible, and rotational spectra to determine molecular structure, bond parameters, functional groups, molecular symmetry, and electronic transitions.

### **Unit I Chemical Thermodynamic II**

**Lecture/ Marks 15**

Need for a Second law; statement of the second law of thermodynamics; Concept of heat reservoirs and heat engines; Carnot cycle; Carnot engine and refrigerator; Kelvin – Planck and Clausius statements and equivalence of the two statements with entropic formulation; Carnot's theorem; Values of  $dQ/T$  and Clausius inequality; Physical concept of Entropy; Entropy is a measure of the microscopic disorder of the system. Entropy changes of systems and surroundings for various processes and transformations, Entropy and unavailable work; Temperature – Entropy diagram, Useful work and The Gibbs and Helmholtz function, Changes at constant T, P. Application to electric work. Criteria for spontaneity and equilibrium, Gibbs- Helmholtz equation, The Gibbs Function and useful work in biological systems, Gibbs free energy and spontaneous phase transition, Maxwell's relations; Joule-Thomson experiment and its consequences; inversion temperature; Joule-Thomson coefficient for a van der Waals gas; General heat capacity relations

### **Unit IV Ionic Equilibrium**

**Lecture Marks 15**

Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect; dissociation constants of mono-, di-and triprotic acids (exact treatment).

Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions; derivation of Henderson equation and its applications; buffer capacity, buffer range, buffer action and applications of buffers in analytical chemistry and biochemical processes in the human body.

Solubility and solubility product of sparingly soluble salts – applications of solubility product principle. Qualitative treatment of acid-base titration curves (calculation of pH at various stages). Theory of acid-base indicators; selection of indicators and their limitations. Multistage equilibria in polyelectrolyte systems; hydrolysis and hydrolysis constants.

### **Unit III Colligative Properties**

**Lecture/ Marks 10**

Thermodynamic derivation using chemical potential to derive relation between the four colligative properties (i) relative lowering of vapour pressure. ii) elevation of boiling point iii) depression of freezing point iv) osmotic pressure) and amount of solute, application in calculating molar masses of normal, associated and dissociated solutes in solution.

Thermochemistry: Heats of reactions, enthalpy of formation of molecules and ions and enthalpy of combustion; Enthalpy of reaction; Hess's law, various types of enthalpy of reactions, calculation of bond energy, bond dissociation energy and resonance energy from thermochemical data, effect of temperature (Kirchhoff's equations) and pressure on enthalpy of reactions. Adiabatic flame temperature, explosion temperature

**Unit IV: Molecular Spectroscopy****Lecture/Marks: 30**

Characterization of electromagnetic radiation, quantization of energy, interaction of matter and radiation, region of spectra, representation of spectra, basic elements of practical spectroscopy, resolving power, factors affecting the width and intensity of spectral transition

Rotation spectroscopy: Selection rules, intensities of spectral lines, determination of bond lengths of diatomic and linear triatomic molecules, isotopic substitution.

Vibrational spectroscopy: Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies, fundamental frequencies, overtones, hot bands, degrees of freedom for polyatomic molecules, modes of molecular vibrations (fundamental and non-fundamental), IR active molecules, fingerprint region and its significance; effect of deuteration; concept of group frequencies. characteristic and diagnostic stretching and bending vibrations frequencies (special examples like C-H, N-H, O-H, C-O, C-N, C-X, C=C, C=O, C=N, N=O, C≡C, C≡N, including skeletal vibrations of aromatic compounds); factors affecting stretching frequencies: effect of conjugation, electronic effects, mass effect, bond multiplicity, ring-size, solvent effect, H-bonding on IR absorptions; application in functional group analysis.

Vibration-rotation spectroscopy: diatomic vibrating rotator, P, Q, R branches.

Raman spectroscopy: Qualitative treatment of Rotational Raman effect; Effect of nuclear spin, Vibrational Raman spectra, Stokes and anti-Stokes lines; their intensity difference, rule of mutual exclusion.

Electronic spectroscopy: Franck-Condon principle, electronic transitions, singlet and triplet states, fluorescence and phosphorescence, dissociation and predissociation, calculation of electronic transitions of polyenes using free electron model.

Types of electronic transitions, end absorption; transition dipole moment and allowed/forbidden transitions; chromophores and auxochromes; Bathochromic and Hypsochromic shifts; intensity of absorptions (Hyper-/Hypochromic effects); application of Woodward's Rules for calculation of  $\lambda_{\max}$  for the following systems: conjugated diene,  $\alpha,\beta$ -unsaturated aldehydes and ketones (alicyclic, homoannular and heteroannular); extended conjugated systems (dienes, aldehydes and ketones); relative positions of  $\lambda_{\max}$  considering conjugative effect, steric effect, solvent effect, effect of pH; effective chromophore concentration: keto-enol systems; benzenoid transitions.

*Suggested readings*

- Atkins, P., de Paula, J., & Keeler, J. *Atkins' Physical Chemistry*, 12th Edition, Oxford University Press.
- Castellan, G. W. *Physical Chemistry*, 3rd Edition, Narosa Publishing House.
- Engel, T., & Reid, P. *Physical Chemistry*, 4th Edition, Pearson Education.
- Levine, I. N. *Physical Chemistry*, 7th Edition, McGraw-Hill Education.
- Puri, B. R., Sharma, L. R., & Pathania, M. S. *Principles of Physical Chemistry*, 48th Edition, Vishal Publishing Co.
- Banwell, C. N., & McCash, E. M. *Fundamentals of Molecular Spectroscopy*, 4th Edition, McGraw-Hill.
- Hollas, J. M. *Modern Spectroscopy*, 4th Edition, John Wiley & Sons.
- Pavia, D. L., Lampman, G. M., Kriz, G. S., & Vyvyan, J. A. *Introduction to Spectroscopy*, 5th Edition, Cengage Learning.

## Semester V

|                              |                                                            |
|------------------------------|------------------------------------------------------------|
| <i>NCrF level</i>            | 5.5                                                        |
| <i>Title of the Course</i>   | <i>Physical Chemistry Practical – I</i>                    |
| <i>Course code</i>           | CHMM-504                                                   |
| <i>Paper credit</i>          | 04 (L 0 – T 0 - P 4)                                       |
| <i>Total Contact Hours</i>   | 120 hours                                                  |
| <i>Distribution of Marks</i> | 100 (End semester examination 70 + internal assessment 30) |

### **Course Objectives**

After successful completion of this course, students will be able to

- To cultivate baseline proficiency in exploring the physical properties of multi-phase liquid systems including surface tension, viscosity, and optical characteristics
- Impart deep functional understandings of instrumental diagnostics encompassing automated pH-metry, conductometry, potentiometry, and polarimetry
- Construct advanced working strategies for studying chemical kinetics, thermodynamic phase behaviors, complexation parameters, and calorimetric operations
- Enable operational execution of quantitative electronic absorption spectroscopy and verify fundamental physical laws governing analytical metrics
- Transition numerical operations towards algorithmic models using automated computer computing frameworks for scientific plotting, least-square fitting, and quantum chemical simulations.

### **Course Outcomes (COs)**

CO1: Characterize physical constants and dynamic properties of liquids via experimental drop configurations, viscometric parameters, and optical rotations

CO2: Perform complex analytical titrations utilizing advanced conductometric, potentiometric, and pH-metric architectures to decode multi-component chemical blends.

CO3: Determine mechanistic rate laws, reaction orders, activation energies, and thermodynamic equilibria parameters governing multi-phase or ionic solutions.

CO4: Execute precise multi-component spectrophotometric calibrations, verify Lambert-Beer's boundaries, compute transition energies, and define structure-absorption matrices.

At least 10 experiments are to be performed from the list of experiments given below:

- To determine the coefficient of viscosity of a given liquid by Ostwald viscometer.
- To determine the composition of a given mixture by viscosity method.
- To determine the surface tension of a liquid by stalagmometer.
- To determine the composition of a given mixture by surface tension method.
- To study the variation of surface tension of aqueous solutions of n-propyl alcohol.
- To determine the mutual solubility curve of phenol and water.

- To determine the molecular mass of a volatile liquid by Victor Meyer's method
- To determine the specific rotation of an optically active substance by polarometric method.
- To determine the specific reaction rate of hydrolysis of methylacetate catalyzed by hydrogen ions at room temperature
- To find the rate of decomposition of  $\text{H}_2\text{O}_2$  catalyzed by  $\text{Fe}^{3+}$  ions.
- To test the validity of Beer-Lambert's law using colorimeter.
- To study the rate of acid catalyzed iodination of acetone.
- To obtain Freundlich isotherm for adsorption of oxalic acid on activated charcoal.
- To study the distribution of iodine between  $\text{CCl}_4$  and water.
- To verify Debye, Huckel, Onsagar equation for sodium chloride.
- To conduct conductometric titrations across targeted systems: (a) strong acid vs. strong base, and (b) weak acid vs. strong base
- To determine the baseline cell constant of a physical conductivity cell to calculate the specific conductance of an electrolyte solution
- To conduct pH-metric titrations across varied systems: (a) strong acid vs. strong base, (b) weak acid vs. strong base, and (c) strong acid vs. weak base
- To map out the 200–500 nm electronic absorption spectra for  $\text{KMnO}_4$  and  $\text{K}_2\text{Cr}_2\text{O}_7$  (dissolved in 0.1 M  $\text{H}_2\text{SO}_4$ ) to locate absolute  $\lambda_{\text{max}}$  configurations. Calculate transition energies across multiple scientific units
- To evaluate the pH-dependence of electronic absorption properties across the UV-Vis spectrum (200–500 nm) for  $\text{K}_2\text{Cr}_2\text{O}_7$  solutions
- To record and analyse the 200–350 nm ultraviolet spectra profiles for organic solvents/molecules (acetone, acetaldehyde, 2-propanol, acetic acid) dissolved in water
- To verify compliance with Lambert-Beer's core operational laws to locate unknown concentrations of  $\text{CuSO}_4$ ,  $\text{KMnO}_4$ , or  $\text{K}_2\text{Cr}_2\text{O}_7$  solutions

*In Examination any two experiment have to performed (35 marks each)*

*Distribution of marks: Theory: Marks 05, Presentation of results including tabulation of data, drawing of graphs, systematic reporting: Marks 15, Completion: Marks 02, Results: Marks 03, Viva: Marks 10*

### **Suggested Readings**

- Viswanathan, B.; Raghavan, P. S., Practical Physical Chemistry, Viva Books, New Delhi (2014)
- Yadav, J. B., Advanced Practical Physical Chemistry, Krishna Prakashan, Meerut (2015).

## Semester VI

|                              |                                                                   |
|------------------------------|-------------------------------------------------------------------|
| <i>NCrF level</i>            | 5.5                                                               |
| <i>Title of the Course</i>   | <i>Inorganic Chemistry – III</i>                                  |
| <i>Course code</i>           | <i>CHMM-601</i>                                                   |
| <i>Paper credit</i>          | <i>04 (L 4 – T 0 - P 0)</i>                                       |
| <i>Total Contact Hours</i>   | <i>70 hours</i>                                                   |
| <i>Distribution of Marks</i> | <i>100 (End semester examination 70 + internal assessment 30)</i> |

### Course Objectives

After successful completion of this course, students will be able to:

- Understand the principles governing the thermodynamic and kinetic stability of coordination compounds and the mechanisms of substitution and electron transfer reactions in transition metal complexes.
- Explain the structure, bonding, nomenclature, synthesis, and reactivity of organometallic compounds with emphasis on metal carbonyls, nitrosyls, alkene, alkyne, allyl, and alkyl complexes.
- Develop a comprehensive understanding of the chemistry of lanthanoids and actinoids, including their electronic structures, magnetic properties, separation techniques, and coordination behaviour.
- Acquire knowledge of systematic qualitative inorganic analysis, including the separation and identification of cations and anions, interfering radicals, and the application of selective organic reagents.
- Apply statistical methods to analyze experimental data, evaluate errors, and assess the accuracy, precision, and reliability of analytical measurements.
- Correlate concepts of coordination chemistry, organometallic chemistry, analytical chemistry, and statistical analysis with applications in catalysis, materials science, environmental chemistry, bioinorganic chemistry, and industrial processes.
- Develop analytical reasoning, quantitative problem-solving ability, and scientific interpretation skills required for advanced studies and research in inorganic chemistry.

### Course Outcomes (COs)

Upon successful completion of the course, students will be able to:

- CO1:** Explain the concepts of thermodynamic and kinetic stability of coordination compounds, evaluate stability constants, chelate effects, and predict the lability and inertness of transition metal complexes.
- CO2:** Interpret substitution mechanisms in octahedral and square-planar complexes, explain the trans effect and electron transfer reactions, and correlate reaction mechanisms with electronic structure and ligand properties.
- CO3:** Describe the structure, bonding, electron counting, nomenclature, synthesis, and reactions of organometallic compounds, including metal carbonyls, nitrosyls, alkene, alkyne, allyl, and alkyl complexes, and apply the 18-electron rule to predict their stability.

**CO4:** Explain the chemistry of lanthanoids and actinoids, including electronic configurations, oxidation states, magnetic and spectral properties, lanthanide contraction, separation techniques, and coordination behaviour.

**CO5:** Apply the principles of qualitative inorganic analysis to systematically identify cations and anions, remove interfering radicals, and utilize selective organic reagents in inorganic analysis.

**CO6:** Perform statistical analysis of experimental data by evaluating different types of errors, significant figures, confidence limits, accuracy, precision, and reliability of analytical results.

#### **Unit I Reaction Mechanism in Coordination chemistry- I**

**Lecture/Marks: 20**

Thermodynamic stability of complexes, stepwise and overall formation constants, factors effecting on stability, Irving-Williams series, kinetic stability, lability and inertness, detection of complex formation, determination of stability constants

Chelate effect, conditions for chelation, enthalpy and entropy aspect of chelate effect, factors effecting stability of chelates, applications in analytical chemistry and biology

Introduction to inorganic reaction mechanisms, Substitution reactions in octahedral complexes, effect of acid and bases on substitution reaction of octahedral complexes, factor affecting the substitution reaction, Interpretation of lability and inertness of transition metal complexes (based on VBT & CFT), factors effecting on lability and inertness.

Substitution reaction of square planar complexes, Trans-effect, theories of trans-effect, trans effect in synthesis of square planar complexes, electron transfer reactions (elementary ideas only)

#### **Unit II Organometallic chemistry I**

**Lecture/Marks: 20**

Definition, classification, haptacity, 18 electron rule, electron count in complex, nature of metal-carbon bond, nomenclature, history and perspective

Metal carbonyls: classifications, bonding, synergic effect, evidences of pi-back bonding, factor effecting stretching frequency, moding modes of carbonyls, number and intensity of IR bands in carbonyls, synthesis and reactions of metal carbonyls

Metal Nitrosyls: structure and bonding

Metal alkenes, alkynes, allyls: Synthesis, Structure and Bonding

Metal Alkyls: Important structural features of methyl lithium (tetramer) and trialkyl aluminium (dimer), concept of multicenter bonding in these compounds, role of triethylaluminium in polymerisation of ethene (Ziegler–Natta Catalyst), Species present in ether solution of Grignard reagent and their structures, Schlenk equilibrium

Fundamentals of organometallic reactions: oxidative addition, reductive elimination, insertion and elimination reaction

#### **Unit IV Inner transition elements**

**Lecture/Marks: 10**

Lanthanoids: Electronic configuration, oxidation states, colour, spectral and magnetic properties, lanthanide contraction, separation of lanthanides (ion-exchange method only), coordination chemistry of lanthanides

Actinoids: electronic configuration, oxidation states, magnetic properties, Comparison with lanthanides

**Unit V Qualitative Inorganic Analysis**

**Lecture/Marks: 15**

Basic principles involved in analysis of cations and anions and solubility products, common ion effect. Principles involved in separation of cations into groups and choice of group reagents. Interfering anions (fluoride, borate, oxalate and phosphate) and need to remove them after Group II

Organic reagent in inorganic analysis: Cupferron, dithizone, benzoin- $\alpha$ -oxime, 1-nitroso-2-naphthol, diphenyl carbazide, diphenyl carbazone, salicylaldehyde, 1,10-phenanthroline, magnesium, thiourea, zinc uranyl acetate, oxine

**Unit VI Statistical analysis of data**

**Lecture/Marks: 05**

Error, types of error, significant figures, accuracy and precision, method of expressing accuracy and precision, confidence limit, distribution of random error, statistical treatment of finite samples

**Suggested reading**

- Huheey, J. E., Keiter, E. A., Keiter, R. L., & Medhi, O. K. *Inorganic Chemistry: Principles of Structure and Reactivity*, 4th Edition, Pearson Education.
- Housecroft, C. E., & Sharpe, A. G. *Inorganic Chemistry*, 5th Edition, Pearson.
- Miessler, G. L., Fischer, P. J., & Tarr, D. A. *Inorganic Chemistry*, 5th Edition, Pearson.
- Cotton, F. A., Wilkinson, G., Murillo, C. A., & Bochmann, M. *Advanced Inorganic Chemistry*, 6th Edition, Wiley.
- Shriver, D. F., Weller, M., Overton, T., Rourke, J., & Armstrong, F. *Shriver and Atkins' Inorganic Chemistry*, 6th Edition, Oxford University Press.
- Crabtree, R. H. *The Organometallic Chemistry of the Transition Metals*, 7th Edition, Wiley.



## Semester VI

|                              |                                                                   |
|------------------------------|-------------------------------------------------------------------|
| <i>NCrF level</i>            | 5.5                                                               |
| <i>Title of the Course</i>   | <i>Organic Chemistry - III</i>                                    |
| <i>Course code</i>           | <i>CHMM-602</i>                                                   |
| <i>Paper credit</i>          | <i>04 (L 4 – T 0 - P 0)</i>                                       |
| <i>Total Contact Hours</i>   | <i>70 hours</i>                                                   |
| <i>Distribution of Marks</i> | <i>100 (End semester examination 70 + internal assessment 30)</i> |

### Course Objectives

After successful completion of this course, students will be able to:

1. Understand the chemistry, synthesis, structure, properties, and reactivity of polynuclear aromatic hydrocarbons, carbonyl compounds, active methylene compounds, and heterocyclic compounds.
2. Explain the mechanisms and synthetic applications of important organic name reactions, heterocyclic syntheses, photochemical reactions, and pericyclic reactions.
3. Develop a comprehensive understanding of molecular orbital concepts governing photochemical and pericyclic reactions, including stereochemistry and regioselectivity.
4. Acquire knowledge of modern spectroscopic techniques such as NMR, ESR, and Mass Spectrometry for structural elucidation of organic compounds.
5. Interpret spectroscopic data to identify molecular structures, functional groups, stereochemistry, and fragmentation patterns.
6. Apply mechanistic reasoning to predict reaction pathways, products, and synthetic strategies in organic chemistry.
7. Develop analytical, problem-solving, and critical thinking skills required for advanced organic synthesis, medicinal chemistry, materials chemistry, and chemical research.

### Course Outcomes (COs)

Upon successful completion of the course, students will be able to

- CO1:** Explain the structure, synthesis, properties, and reactions of polynuclear aromatic hydrocarbons, carbonyl compounds, and active methylene compounds, and interpret their synthetic importance.
- CO2:** Describe the mechanisms and synthetic applications of important organic transformations, including Aldol, Benzoin, Knoevenagel, Claisen-Schmidt, Perkin, Cannizzaro, Beckmann, Benzil-Benzilic acid rearrangement, Haloform, and Michael addition reactions.
- CO3:** Explain the synthesis, structure, aromaticity, reactivity, and mechanistic aspects of important heterocyclic compounds including pyrrole, furan, thiophene, pyridine, indole, quinoline, and isoquinoline.
- CO4:** Apply Frontier Molecular Orbital (FMO) theory to explain photochemical and pericyclic reactions, including electrocyclic reactions, cycloadditions, sigmatropic rearrangements, and their stereochemical outcomes.
- CO5:** Interpret proton NMR spectra by analyzing chemical shifts, spin-spin coupling, integration, anisotropic effects, proton equivalence, and first-order splitting patterns for structural elucidation of organic compounds.

**CO6:** Explain the principles and applications of ESR and Mass Spectrometry, interpret fragmentation patterns, molecular ion peaks, and McLafferty rearrangements for molecular structure determination.

**CO7:** Solve numerical and conceptual problems involving reaction mechanisms, heterocyclic chemistry, photochemistry, pericyclic reactions, and spectroscopic techniques, and apply these concepts to modern organic synthesis, medicinal chemistry, materials science, and chemical research.

### **Unit II Polynuclear Hydrocarbons and Carbonyl Compounds**

**Lecture Marks 15**

Polynuclear Hydrocarbons: Structures, preparations and reactions of naphthalene, phenanthrene and anthracene.

Carbonyl Compounds: Structure, preparation and reactivity; nucleophilic addition-elimination reactions with ammonia derivatives and their mechanisms.

Active Methylene Compounds: Keto-enol tautomerism. Preparation and synthetic applications of diethyl malonate and ethyl acetoacetate.

Name Reactions: Mechanisms of Aldol and Benzoin condensation, Knoevenagel condensation, Claisen-Schmidt, Perkin and Cannizzaro reaction, Beckmann and benzil-benzilic acid rearrangements, haloform reaction and Michael addition

### **Unit-II: Heterocyclic chemistry**

**Lecture/Marks: 15**

Polynuclear hydrocarbons and their derivatives: synthetic methods include Haworth, Bardhan-Sengupta, Bogert-Cook and other useful syntheses (with mechanistic details); fixation of double bonds and Fries rule; reactions (with mechanism) of naphthalene, anthracene and phenanthrene and their derivatives. Heterocyclic compounds: Biological importance of heterocycles referred in the syllabus; 5- and 6-membered rings with one heteroatom; reactivity, orientation and important reactions (with mechanism) of furan, pyrrole, thiophene and pyridine; synthesis (including retrosynthetic approach and mechanistic details): pyrrole: Knorr synthesis, Paal-Knorr synthesis, Hantzsch; furan: Paal-Knorr synthesis, Feist-Benary synthesis and its variation; thiophenes: Paal-Knorr synthesis, Hinsberg synthesis; pyridine: Hantzsch synthesis; benzo-fused 5-and 6-membered rings with one heteroatom: reactivity, orientation and important reactions (with mechanistic details) of indole, quinoline and isoquinoline; synthesis (including retrosynthetic approach and mechanistic details): indole: Fischer, quinoline: Skraup, isoquinoline: Bischler Napieralski synthesis.

### **Unit-II: Photochemistry and pericyclic reactions**

**Lecture/Marks: 15**

Electron excitation in organic molecules (alkenes and carbonyl compounds); fate of electronically excited molecules; singlet and triplet states; photoreduction of carbonyl compounds; photoaddition of alkenes to carbonyl compounds (Paterno-Buchi reaction); photoaddition of alkenes to aromatic compounds; photorearrangement (cis-trans isomerization, intramolecular cyclization of dienes); photochemical fragmentation (photolysis of carbonyl compounds: Norrish type I and type II reactions).

Mechanism, stereochemistry, regioselectivity

Electrocyclic reactions: FMO approach involving  $4\pi$ - and  $6\pi$ -electrons (thermal and photochemical) and corresponding cycloreversion reactions.

Cycloaddition reactions: FMO approach, Diels-Alder reaction, photochemical [2+2] cycloadditions.

Sigmatropic reactions: FMO approach, sigmatropic shifts and their order; [1,3] and [1,5] H shifts and [3,3] shifts with reference to Claisen and Cope rearrangements.

## **Unit-II: NMR spectroscopy and Mass Spectrometry**

**Lecture/Marks: 25**

NMR Spectroscopy: Introduction; nuclear spin; NMR active molecules; basic principles of Proton Magnetic Resonance; choice of solvent and internal standard; equivalent and non-equivalent protons; chemical shift and factors influencing it; ring current effect; significance of the terms: up-/downfield, shielded and deshielded protons; spin coupling and coupling constant (1st order spectra); relative intensities of first-order multiplets: Pascal's triangle; chemical and magnetic equivalence in NMR ; anisotropic effects in alkene, alkyne, aldehydes and aromatics; NMR peak area, integration; relative peak positions with coupling patterns of common organic compounds (both aliphatic and benzenoid-aromatic); rapid proton exchange; interpretation of NMR spectra of simple compounds

Electron spin resonance (ESR) spectroscopy and its principle, characteristic features of ESR spectra, line shapes and line widths hyperfine structure, ESR of simple free radicals, and copper (II) compounds

Mass Spectroscopy: Mass spectral fragmentation of organic compounds, common functional groups; molecular peak, McLafferty rearrangements, examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Applications of IR, UV and NMR spectroscopy for identification of simple organic molecules

### Suggested Reading

- Clayden, J., Greeves, N., & Warren, S. *Organic Chemistry*, 2nd Edition, Oxford University Press.
- Solomons, T. W. G., Fryhle, C. B., & Snyder, S. A. *Organic Chemistry*, 13th Edition, Wiley.
- Morrison, R. T., & Boyd, R. N. *Organic Chemistry*, 7th Edition, Pearson Education.
- Smith, M. B. *March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure*, 8th Edition, Wiley.
- Joule, J. A., Mills, K., & Smith, G. F. *Heterocyclic Chemistry*, 5th Edition, Wiley.
- Pavia, D. L., Lampman, G. M., Kriz, G. S., & Vyvyan, J. A. *Introduction to Spectroscopy*, 5th Edition, Cengage Learning.
- Silverstein, R. M., Webster, F. X., Kiemle, D. J., & Bryce, D. L. *Spectrometric Identification of Organic Compounds*, 9th Edition, Wiley.
- Kemp, W. *Organic Spectroscopy*, 3rd Edition, Palgrave Macmillan.
- Banwell, C. N., & McCash, E. M. *Fundamentals of Molecular Spectroscopy*, 4th Edition, McGraw-Hill.

## Semester VI

|                              |                                                                   |
|------------------------------|-------------------------------------------------------------------|
| <i>NCrF level</i>            | 5.5                                                               |
| <i>Title of the Course</i>   | <i>Physical Chemistry - III</i>                                   |
| <i>Course code</i>           | <i>CHMM-603</i>                                                   |
| <i>Paper credit</i>          | <i>04 (L 4 – T 0 - P 0)</i>                                       |
| <i>Total Contact Hours</i>   | <i>70 hours</i>                                                   |
| <i>Distribution of Marks</i> | <i>100 (End semester examination 70 + internal assessment 30)</i> |

### Course Objectives

After successful completion of this course, students will be able to:

- Develop a comprehensive understanding of the principles of electrochemistry, conductance, solid-state chemistry, photochemistry, and quantum mechanics.
- Explain the theories of electrolytic conductance, ionic transport, electrochemical cells, electrode potentials, and their applications in chemical systems.
- Understand the structural features of crystalline solids, symmetry elements, crystal systems, Bravais lattices, and the principles of X-ray diffraction.
- Acquire knowledge of the fundamental principles of photochemistry, including electronic excitation, quantum yield, photochemical reactions, fluorescence, phosphorescence, and their applications.
- Understand the basic principles of quantum mechanics and apply Schrödinger wave mechanics to simple chemical systems such as harmonic oscillators, rigid rotators, and hydrogen-like atoms.
- Apply mathematical and theoretical concepts to solve problems related to electrochemistry, crystal structures, spectroscopy, and quantum chemistry.
- Develop analytical reasoning and quantitative problem-solving skills required for advanced studies in physical chemistry, materials science, spectroscopy, nanoscience, and computational chemistry.

### Course Outcomes (COs)

Upon successful completion of the course, students will be able to

- CO1:** Explain the theories of electrolytic dissociation, ionic conductance, ionic mobility, transference number, and electrochemical cells, and apply these concepts to analyze electrolyte behaviour in solution.
- CO2:** Apply electrochemical principles to determine electrode potentials, EMF, activity coefficients, equilibrium constants, and conductometric and potentiometric titration curves.
- CO3:** Describe the structural characteristics of crystalline solids, explain crystal symmetry, Miller indices, crystal systems, Bravais lattices, and interpret X-ray diffraction using Bragg's law.
- CO4:** Explain the fundamental concepts of photochemistry, including quantum yield, photochemical reactions, photosensitization, fluorescence, and Jablonski diagrams.
- CO5:** Apply the principles of quantum mechanics to describe vibrational motion using the harmonic oscillator model and rotational motion using the rigid rotator model of diatomic molecules.
- CO6:** Explain the quantum mechanical treatment of hydrogen and hydrogen-like atoms, including Schrödinger wave equations, wave functions, quantized energy levels, and electron probability distributions.
- CO7:** Solve numerical and conceptual problems related to conductance, electrochemical cells, crystal structures, photochemical processes, and quantum mechanical models

**Unit I Conductance and Electrochemistry****Lecture Marks 20**

Arrhenius theory of electrolytic dissociation, Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes, Molar conductivity at infinite dilution, Kohlrausch law of independent migration of ions, Debye-Hückel-Onsager equation, Ionic velocities, mobilities and their determinations, transference numbers and their relation to ionic mobilities, determination of transference numbers using Hittorf and Moving Boundary methods, Applications of conductance measurement: (i) degree of dissociation of weak electrolytes, (ii) ionic product of water (iii) solubility and solubility product of sparingly soluble salts, (iv) conductometric titrations, and (v) hydrolysis constants of salts.

Chemical cells, reversible and irreversible cells, with examples, Electromotive force of a cell and its measurement, Nernst equation; Standard electrode (reduction) potential and its application to different kinds of half-cells; Application of EMF measurements in determining (i) free energy, enthalpy and entropy of a cell reaction, (ii) equilibrium constants, and (iii) pH values using hydrogen, quinone-hydroquinone, glass and  $\text{SbO/Sb}_2\text{O}_3$  electrodes. Concentration cells with and without transference, liquid junction potential, determination of activity coefficients and transference numbers. Qualitative discussion of potentiometric titrations (acid-base, redox, precipitation)

**Unit II Solid State-II****Lecture/Marks: 10**

Nature of the solid state, law of constancy of interfacial angles, law of rational indices, Miller indices, elementary ideas of symmetry, symmetry elements and symmetry operations, qualitative idea of point and space groups, seven crystal systems and fourteen Bravais lattices; X-ray diffraction, Bragg's law.

**Unit IV Fundamentals of Photochemistry****Lecture Marks 15**

Characteristics of electromagnetic radiation, Lambert-Beer's law and its limitations, and the physical significance of absorption coefficients. Laws of photochemistry, quantum yield, actinometry, examples of low and high quantum yields, photochemical equilibrium and the differential rate of photochemical reactions, photosensitised reactions, and quenching. Role of photochemical reactions in biochemical processes, photostationary states, Jablonski diagram, simple ideas of fluorescence, phosphorescence, and chemiluminescence.

**Unit IV Quantum Mechanics-III****Lecture Marks 25**

Qualitative treatment of simple harmonic oscillator model of vibrational motion: Setting up of Schrödinger equation and discussion of solution and wave functions; normalization of wave functions. Vibrational energy of diatomic molecules and zero-point energy

Rigid rotator model of rotation of diatomic molecule: Schrödinger equation; transformation to spherical polar coordinates. Separation of variables; spherical harmonics and discussion of solution

Qualitative treatment of hydrogen atom and hydrogen-like ions: setting up of Schrödinger equation in spherical polar coordinates; radial part; quantization of energy (only final energy expression). Average, root mean square and most probable distances of electron from nucleus

### Suggested Reading

- Atkins, P., de Paula, J., & Keeler, J. *Atkins' Physical Chemistry*, 12th Edition, Oxford University Press.
- Levine, I. N. *Physical Chemistry*, 7th Edition, McGraw-Hill Education.
- Engel, T., & Reid, P. *Physical Chemistry*, 4th Edition, Pearson Education.
- Castellan, G. W. *Physical Chemistry*, 3rd Edition, Narosa Publishing House.
- Puri, B. R., Sharma, L. R., & Pathania, M. S. *Principles of Physical Chemistry*, 48th Edition, Vishal Publishing Co.
- Bard, A. J., & Faulkner, L. R. *Electrochemical Methods: Fundamentals and Applications*, 2nd Edition, Wiley.
- Bockris, J. O'M., & Reddy, A. K. N. *Modern Electrochemistry*, Springer.
- West, A. R. *Solid State Chemistry and Its Applications*, 2nd Edition, Wiley.
- Smart, L., & Moore, E. *Solid State Chemistry: An Introduction*, 4th Edition, CRC Press.
- McQuarrie, D. A. *Quantum Chemistry*, University Science Books.
- Atkins, P. W., & Friedman, R. S. *Molecular Quantum Mechanics*, 6th Edition, Oxford University Press.
- Levine, I. N. *Quantum Chemistry*, 7th Edition, Pearson.
- Rohatgi-Mukherjee, K. K. *Fundamentals of Photochemistry*, New Age International.
- Turro, N. J., Ramamurthy, V., & Scaiano, J. C. *Modern Molecular Photochemistry of Organic Molecules*, University Science Books.
- Glasstone, S. *An Introduction to Electrochemistry*, East-West Press.
- Kittel, C. *Introduction to Solid State Physics*, 8th Edition, Wiley.

## Semester VI

|                              |                                                            |
|------------------------------|------------------------------------------------------------|
| <i>NCrF level</i>            | 5.5                                                        |
| <i>Title of the Course</i>   | <i>Inorganic Chemistry Practical - I</i>                   |
| <i>Course code</i>           | CHMM-604                                                   |
| <i>Paper credit</i>          | 04 (L 0 – T 0 - P 4)                                       |
| <i>Total Contact Hours</i>   | 120 hours                                                  |
| <i>Distribution of Marks</i> | 100 (End semester examination 70 + internal assessment 30) |

### Course Objectives

Upon completion of this course, the students will be able to:

- Develop a thorough understanding of the principles and systematic procedures involved in qualitative inorganic analysis of simple and complex salt mixtures.
- Acquire practical skills in the identification and separation of cationic and anionic radicals, including insoluble salts and interfering ions, using classical analytical methods.
- Apply volumetric, gravimetric, complexometric, precipitation, and redox analytical techniques for the quantitative estimation of inorganic ions in single- and multi-component systems.
- Understand the principles and applications of chromatographic and colorimetric methods for the separation, identification, and estimation of inorganic species.
- Develop accuracy in laboratory measurements, data recording, error analysis, interpretation of analytical results, and scientific reporting.
- Demonstrate Good Laboratory Practices (GLP), laboratory safety, ethical conduct, and proper handling of analytical chemicals and instruments.

### Course Outcomes (COs)

After successful completion of the course, students will be able to:

- CO1:** Systematically identify cationic and anionic radicals present in complex inorganic salt mixtures by applying the principles of qualitative inorganic analysis.
- CO2:** Explain the chemistry involved in precipitation, complex formation, oxidation-reduction, hydrolysis, and solubility equilibria governing qualitative analysis.
- CO3:** Perform quantitative estimation of inorganic ions using volumetric, gravimetric, precipitation, complexometric, and redox analytical methods with acceptable analytical accuracy.
- CO4:** Separate and estimate individual ions present in binary mixtures using appropriate analytical procedures and calculations.
- CO5:** Carry out chromatographic separation of inorganic ions using paper and thin-layer chromatography (TLC) and interpret chromatographic data.
- CO6:** Determine the concentration of coloured inorganic species using colorimetric techniques through calibration curve preparation and quantitative analysis.
- CO7:** Analyze experimental observations, perform calculations, estimate experimental errors, and prepare scientific laboratory reports.
- CO8:** Demonstrate competence in laboratory safety, Good Laboratory Practices (GLP), scientific ethics, teamwork, and responsible handling of chemicals and analytical instruments.



**Unit I Qualitative Inorganic salt analysis****60 hours**

Analysis of a mixture of salts containing total of four cations and anions including insoluble salts and interfering anions, Emphasis should be given to the understanding of the chemistry of different reactions. Spot tests may be included for cations and anions. Mixtures of radicals should be given so that students have idea on the influence of one radical on another radical.

Cation Radicals:  $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Ca}^{2+}$ ,  $\text{Sr}^{2+}$ ,  $\text{Ba}^{2+}$ ,  $\text{Al}^{3+}$ ,  $\text{Cr}^{3+}$ ,  $\text{Mn}^{2+}/\text{Mn}^{4+}$ ,  $\text{Fe}^{3+}$ ,  $\text{Co}^{2+}/\text{Co}^{3+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Pb}^{2+}$ ,  $\text{Cd}^{2+}$  (Demo),  $\text{Bi}^{3+}$  (Demo),  $\text{Sn}^{2+}/\text{Sn}^{4+}$ ,  $\text{As}^{3+}/\text{As}^{5+}$ ,  $\text{Sb}^{3+}/\text{Sb}^{5+}$  (Demo),  $\text{NH}_4^+$ ,  $\text{Mg}^{2+}$  (Demo).

Anion Radicals:  $\text{Cl}^-$ ,  $\text{Br}^-$ ,  $\text{BrO}_3^-$ ,  $\text{I}^-$ ,  $\text{IO}_3^-$ ,  $\text{SCN}^-$ ,  $\text{S}^{2-}$ ,  $\text{SO}_4^{2-}$ ,  $\text{NO}_3^-$ ,  $\text{NO}_2^-$ ,  $\text{PO}_4^{3-}$ ,  $\text{BO}_3^{3-}$ ,  $\text{CrO}_4^{2-}$  /  $\text{Cr}_2\text{O}_7^{2-}$ ,  $\text{Fe}(\text{CN})_6^{4-}$ ,  $\text{Fe}(\text{CN})_6^{3-}$ .

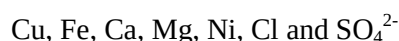
Insoluble Materials:  $\text{Al}_2\text{O}_3$ ,  $\text{Fe}_2\text{O}_3$ ,  $\text{Cr}_2\text{O}_3$ ,  $\text{SnO}_2$ ,  $\text{SrSO}_4$ ,  $\text{BaSO}_4$ ,  $\text{CaF}_2$

Marks distribution: Physical properties and solubility: 2 marks, Preliminary Dry tests: 4 marks, Dry test for acid radicals: 4 marks, Wet test for acid radical: 4 marks, Confirmatory test: 2 marks, Group analysis: 10 marks, Conclusion and remarks ( $3 \times 4 = 10$ ) 12 marks, overall cleanliness: 2 marks, Total = 40 marks

**Unit II Inorganic Quantitative Analysis****40 hours**

Estimation of inorganic ions by volumetric, complexometric, gravimetric, redox and precipitation methods

The following one-component systems should be estimated first:



This should be followed by separation and estimation of individual ions in two-component systems.

- Cu and Fe
- Fe and Ca
- Ca and Mg
- Cu and Ni
- $\text{Cl}^-$  and  $\text{SO}_4^{2-}$ .

(Any one of the above mixtures will be given for estimation in examination.

Marks distribution: Theory: 5 marks, Preparation of standard solution and standardization: 10 marks. Separation of components: 10 marks, Completion of the experiment: 5 mark and Results: 10 marks=Total 40 marks

**Unit III Chromatographic separation****10 hours**

Paper chromatographic separation of Group I, II and III cations by paper/TLC

Marks distribution: Theory: 5 marks, Presentation and Tabulation of data: 5 marks, Development of chromatogram: 8 marks, Completion and result: 2 marks, Total= 20 marks

**Unit III Colorimetric estimation****10 hours**

Colorimetric estimation of Copper, Iron and Nickel,  $\text{KMnO}_4$ ,  $\text{K}_2\text{Cr}_2\text{O}_7$

Marks distribution: Theory: 5 marks, Preparation of standard solution and standardization curve: 10 marks, Result: 5 marks, Total= 20 marks

**Suggested reading**

- Svehla, G., *Vogel's Qualitative Inorganic Analysis*, Pearson Education, 2012.2.
- *Practical Workbook Chemistry (Honours)*, UGBS, Chemistry, University of Calcutta, 2015
- R. L. Madan. *Practical Chemistry*. S. Chand Publishing
- Chatwal, G. R., & Anand, S. *Instrumental Methods of Chemical Analysis*. Himalaya Publishing House.

## Semester VII

|                              |                                                                   |
|------------------------------|-------------------------------------------------------------------|
| <i>NCrF level</i>            | 6.0                                                               |
| <i>Title of the Course</i>   | <i>Advanced Inorganic Chemistry - I</i>                           |
| <i>Course code</i>           | <i>CHMM-701</i>                                                   |
| <i>Paper credit</i>          | <i>04 (L 4 – T 0 - P 0)</i>                                       |
| <i>Total Contact Hours</i>   | <i>70 hours</i>                                                   |
| <i>Distribution of Marks</i> | <i>100 (End semester examination 70 + internal assessment 30)</i> |

### Course Objectives

Upon successful completion of this course, students will be able to:

- Develop an advanced understanding of the mechanisms of substitution, isomerization, and electron transfer reactions in coordination compounds and correlate reaction pathways with kinetic and stereochemical evidence.
- Explain advanced bonding theories of coordination compounds, including Ligand Field Theory (LFT) and Molecular Orbital Theory (MOT), and interpret their electronic spectra using Tanabe–Sugano diagrams, Racah parameters, and nephelauxetic effects.
- Acquire comprehensive knowledge of organometallic chemistry involving metal carbonyls, carbenes, metallocenes, metal arene complexes, and homogeneous catalysis, with emphasis on their synthesis, bonding, structure, reactivity, and applications.
- Understand the crystal structures, bonding, and properties of important inorganic solids and relate lattice energy to their physical and chemical behaviour.
- Explain the structure, function, and catalytic roles of biologically important metal-containing enzymes and metalloproteins involved in essential biological processes.
- Develop analytical, problem-solving, and scientific reasoning skills for interpreting reaction mechanisms, spectroscopic data, structural features, and contemporary applications of inorganic chemistry.

### Course Outcomes (COs)

After successful completion of the course, students will be able to:

- CO1:** Explain the mechanisms of substitution, hydrolysis, aquation, anation, isomerization, racemization, and electron transfer reactions in coordination complexes using kinetic and stereochemical evidence.
- CO2:** Apply Ligand Field Theory and Molecular Orbital Theory to explain bonding, magnetic properties, electronic spectra, Racah parameters, nephelauxetic effect, charge transfer transitions, and crystal field stabilization energies of coordination compounds.
- CO3:** Explain the synthesis, bonding, structure, reactivity, fluxional behaviour, and catalytic applications of organometallic compounds, including metal carbonyls, metal carbenes, metallocenes, and metal arene complexes.
- CO4:** Interpret spectroscopic evidence (UV–Visible, EPR, and multinuclear NMR) for elucidating the structure and dynamics of inorganic and organometallic compounds.
- CO5:** Describe the crystal structures, lattice energies, and structure–property relationships of important inorganic solids.
- CO6:** Explain the structure and biological functions of metalloproteins and metalloenzymes involved in photosynthesis, nitrogen fixation, oxidation, reduction, and coenzyme-mediated biochemical reactions.

**Unit I Reaction Mechanism in Coordination chemistry- II****Lecture/Marks: 20**

Substitution reactions in octahedral complexes, Evidences for dissociative mechanism, water exchange, anation, aquation or hydrolysis (details of rate equation), factors affecting in acid hydrolysis, stereochemistry of acid catalysed reaction, isomerization and racemization of octahedral complexes, substitution reaction without breaking metal-ligand bond

Substitution reaction in square planar complexes, factors affecting rates of substitution reaction, mechanism of substitution reaction of square planar complexes, evidences in favour of associative mechanism, application of trans effect

Electron transfer reaction, outer-sphere and inner-sphere mechanism, salient features of these mechanism, Cross reaction, Marcus theorem, acceleration of rate of electron transfer reaction, inner-sphere reaction of complex with organic ligand, successor complex and fission, redox reaction with two electron involvement, complementary and non-complementary reaction, use of electron transfer reactions for synthesising complexes

**Unit II Bonding theories and Electronic spectra of coordination Complex****Lecture/Marks: 15**

Demerits of CFT, nephelauxetic effect and EPR evidences, Racah parameters, Ligand field theory, Molecular orbital theory, charge transfer spectra, Tanabe sugano diagram, and calculation of B and CFSE

**Unit III Organometallic chemistry II: Carbene and catalysis****Lecture/Marks: 15**

Metal carbonylate ions: synthesis, properties and reactions

Metal carbonyl hydrides: synthesis, properties, bonding modes and spectral properties M-H bond

Metal carbonyl halides: synthesis and reactions

Fluxionality in organometallic compounds and spectral evidences ( $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{31}\text{P}$  NMR)

Metal carbenes: Introduction to metal-carbon multiple bonds, classifications, Fischer carbene, Schrock carbene, (Synthesis, Structure, bonding, synthesis and application), Tebb's reagent metal carbynes

Bonding in cyclobutadiene, cyclopentadiene

Ferrocene: Preparation and reactions (acetylation, alkylation, nitration and halogenation, metallation, Mannich condensation). Structure and aromaticity, Comparison of aromaticity and reactivity with that of benzene, other metallocenes

Metal arene complexes: Synthesis, properties, reactions

**Unit IV Inorganic solid****Lecture/Marks: 10**

Characteristic structure types of ionic solids: CsCl, NaCl, Spalerite and Wurtzite types of ZnS, fluorite and anti-fluorite, nickel arsenide,  $\text{CdCl}_2$ ,  $\text{CdI}_2$ , rutile, perovskite and spinels, Lattice enthalpy, consequences of lattice enthalpy

**Unit V Bioinorganic Chemistry IV****Lecture/Marks: 10**

Photosynthesis: reaction pathway, role of magnesium ions

Active site structure and activity of nitrogenase enzyme, xanthine oxidase, alcohol dehydrogenase, aldehyde oxidase, aldehyde dehydrogenase and V-B<sub>12</sub>

### Suggested reading

- F. A. Cotton, G. Wilkinson, C. A. Murillo & M. Bochmann, *Advanced Inorganic Chemistry*, 6th Edition, Wiley.
- J. E. Huheey, E. A. Keiter & R. L. Keiter, *Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson.
- Miessler, Fischer & Tarr, *Inorganic Chemistry*, 5th Edition, Pearson.
- Gary L. Miessler, Paul J. Fischer & Donald A. Tarr, *Inorganic Chemistry*, Pearson.
- Shriver, D. F., Weller, M., Overton, T., Rourke, J. & Armstrong, F., *Inorganic Chemistry*, Oxford University Press.
- Satya Prakash, G. D. Tuli, S. K. Basu & R. D. Madan, *Advanced Inorganic Chemistry*, S. Chand.
- P. L. Soni & Mohan Katyal, *Textbook of Inorganic Chemistry*, Sultan Chand & Sons.
- R. L. Dutta, *Inorganic Chemistry*, Part I & II, New Age International.
- Gurdeep Raj, *Advanced Inorganic Chemistry*, Goel Publishing House.
- B. R. Puri, L. R. Sharma & K. C. Kalia, *Principles of Inorganic Chemistry*, Vishal Publishing Co.
- A. K. De, *A Textbook of Inorganic Chemistry*, New Age International.

## Semester VII

|                              |                                                            |
|------------------------------|------------------------------------------------------------|
| <i>NCrF level</i>            | 6.0                                                        |
| <i>Title of the Course</i>   | <i>Advanced Organic Chemistry - I</i>                      |
| <i>Course code</i>           | CHMM-702                                                   |
| <i>Paper credit</i>          | 04 (L 4 – T 0 - P 0)                                       |
| <i>Total Contact Hours</i>   | 70 hours                                                   |
| <i>Distribution of Marks</i> | 100 (End semester examination 70 + internal assessment 30) |

### Course Objectives

Upon successful completion of this course, students will be able to:

- Develop an advanced understanding of selective oxidation and reduction reactions, their mechanisms, reagent chemistry, stereochemical aspects, and synthetic applications in organic chemistry.
- Explain the mechanisms of important molecular rearrangements involving carbon, oxygen, nitrogen, and aromatic systems, and predict the products based on mechanistic pathways.
- Acquire comprehensive knowledge of the synthesis, properties, reactions, stereochemistry, and analytical aspects of amino acids, peptides, and nucleic acids.
- Apply mechanistic concepts to design efficient synthetic routes using appropriate oxidizing agents, reducing agents, and rearrangement reactions.
- Correlate reaction mechanisms with regioselectivity, chemoselectivity, stereoselectivity, and reaction conditions in modern organic synthesis.
- Develop problem-solving skills for interpreting reaction mechanisms, retrosynthetic analysis, and biomolecular transformations relevant to research, pharmaceutical chemistry, and chemical industries.

### Course Outcomes (COs)

After successful completion of the course, students will be able to:

- CO1:** Explain the mechanisms, selectivity, and applications of important oxidation reactions using transition metal-, DMSO-, selenium-, and peroxide-based oxidizing reagents.
- CO2:** Select suitable oxidizing or reducing reagents for the chemoselective transformation of functional groups and predict reaction products under different conditions.
- CO3:** Describe the mechanisms and synthetic applications of catalytic hydrogenation, dissolving metal reductions, hydride reductions, borane reductions, and other important reduction reactions.
- CO4:** Analyze the mechanisms of molecular rearrangements involving carbon-, oxygen-, nitrogen-, and aromatic-centered migrations and apply them in synthetic organic chemistry.
- CO5:** Explain the synthesis, stereochemistry, properties, and reactions of amino acids and peptides, including modern peptide synthesis and sequence determination techniques.
- CO6:** Describe the structure, chemistry, hydrolysis, and biological significance of nucleic acids and explain the molecular basis of DNA structure and complementary base pairing.
- CO7:** Interpret reaction mechanisms, stereochemical outcomes, and synthetic strategies to solve advanced problems in organic synthesis.

**Unit I: Oxidations****Lecture/Marks: 15**

Oxidation of alcohols to aldehydes/ketones/carboxylic acids: Transition metal-based oxidants: Jones reagent, Collins Reagent, PCC, PDC,  $\text{KMnO}_4$ ,  $\text{MnO}_2$ ,  $\text{Mn}(\text{OAc})_3$ ,  $\text{RuCl}_3/\text{NaIO}_4$  ( $\text{RuO}_4$ ). Dimethyl sulfoxide-based oxidation: Moffatt-Pfitzner Oxidation, Parikh-Doering Oxidation, Corey-Kim Oxidation, Swern Oxidation.

Oxidation of alkenes/alkynes: Ozonolysis,  $\text{KMnO}_4$ , Prévost dihydroxylation, Woodward dihydroxylation, epoxidation by peroxy acids and related reagents

Other oxidation processes: Allylic oxidation by  $\text{SeO}_2$ , Oxidation of aldehydes/ketones by  $\text{SeO}_2$ , Cleavage of 1,2-diols, Hunsdiecker reaction.

**Unit II: Reductions****Lecture/Marks: 15**

Hydrogenation:  $\text{H}_2/\text{Pd-C}$ ,  $\text{H}_2/\text{Lindlar Catalyst}$ ,  $\text{H}_2/\text{Wilkinson's Catalyst}$ , transfer hydrogenation, diimide reduction.

Dissolving Metal Reductions for: alkynes, aldehydes/ketones, esters,  $\alpha,\beta$ -unsaturated ketones, aromatic compounds (Birch reduction), Clemmensen Reduction.

Aluminium-based reagents: lithium aluminum hydride (LAH), lithium trimethoxyaluminium hydride (LTBA), lithium tri-(tert-butoxy)aluminium hydride (LTBA), sodium bis(2-methoxyethoxy)aluminium hydride (Red-Al), selectrides, diisobutylaluminium hydride, alane. Boron-based reagents: Sodium borohydride, Zinc borohydride, Lithium borohydride, Sodium cyanoborohydride, Sodium triacetoxyborohydride, borane.

Other reduction processes: Wolff-Kishner reduction, Clemmensen Reduction, MPV reduction.

**Unit III: Rearrangements****Lecture/Marks: 20**

Rearrangement to electron-deficient carbon: Wagner-Meerwein rearrangement, pinacol pinacolone and related rearrangements, dienone-phenol rearrangement, benzil-benzilic acid rearrangement.

Rearrangement to electron-deficient oxygen: Baeyer-Villiger oxidation, hydroperoxide rearrangement cumene hydroperoxide-phenol rearrangement, Dakin reaction.

Rearrangement to electron-deficient nitrogen (Beckmann rearrangement, Schmidt rearrangement, Hofmann rearrangement, Lossen rearrangement, Curtius rearrangement)

Aromatic rearrangements: Migration from oxygen to ring carbon (Fries rearrangement, Claisen rearrangement), migration from nitrogen to ring carbon (Hofmann-Martius rearrangement, Fischer-Hepp rearrangement, N-azo to C-azo rearrangement, Bamberger rearrangement, Orton rearrangement, Benzidine rearrangement)

**Unit-IV: Amino acids****Lecture/Marks: 20**

Amino acids: Synthesis with mechanistic details: Strecker, Gabriel; acetamido malonic ester, azlactone, Bücherer hydantoin synthesis, synthesis involving diketopiperazine, isoelectric point, zwitterions; electrophoresis, reaction (with mechanism): ninhydrin reaction, Dakin-West reaction; resolution of racemic amino acids.

Peptides: peptide linkage and its geometry; syntheses (with mechanistic details) of peptides using N-protection & C-protection, solid-phase (Merrifield) synthesis; peptide sequence: C-terminal and N-terminal unit determination (Edman, Sanger and 'dansyl' methods); partial hydrolysis; specific cleavage of peptides; use of CNBr.

Nucleic acids: pyrimidine and purine bases (only structure & nomenclature); nucleosides and nucleotides corresponding to DNA and RNA; mechanism for acid catalyzed hydrolysis of nucleosides (both pyrimidine and purine types); comparison of alkaline hydrolysis of DNA and RNA; elementary idea of double helical structure of DNA (Watson-Crick model); complimentary base-pairing in DNA.

### Suggested reading

- Smith, M. B.; March, J., *March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure*, 7th Ed., Wiley India, New Delhi (2015).
- Smith, M. B., *Organic Synthesis*, 4th Ed., Academic Press, Cambridge, Massachusetts (2016).
- Greeves, N.; Clayden, J.; Warren, S., *Organic Chemistry*, 2nd Ed., Oxford University Press, New Delhi (2012).
- Carruthers, W., *Modern Methods of Organic Synthesis*, 4th Ed., Cambridge University Press, New Delhi (2005).
- Zweifel, G. S.; Nantz, M. H.; Somfai, P., *Modern Organic Synthesis: An Introduction*, 2nd Ed., Wiley-Blackwell, New York (2017)
- D. L. Nelson, M. M. Cox, *Lehninger Principles of Biochemistry*; 5th edition, 2008 (W. H. Freeman & Co.).
- R. H. Abeles, P. A. Frey, W. P. Jencks, *Biochemistry*, Jones and Bartlett Publishers, Boston, 1992.
- D. Voet, J. G. Voet, C. W. Pratt, *Fundamentals of Biochemistry: Life at the Molecular Level*, 4th Edition, 2012.



## Semester VII

|                              |                                                            |
|------------------------------|------------------------------------------------------------|
| <i>NCrF level</i>            | 6.0                                                        |
| <i>Title of the Course</i>   | <i>Advanced Physical Chemistry - I</i>                     |
| <i>Course code</i>           | CHMM-702                                                   |
| <i>Paper credit</i>          | 04 (L 4 – T 0 - P 0)                                       |
| <i>Total Contact Hours</i>   | 70 hours                                                   |
| <i>Distribution of Marks</i> | 100 (End semester examination 70 + internal assessment 30) |

### Course Objectives

Upon successful completion of this course, students will be able to:

- Develop an advanced understanding of the principles governing chemical kinetics, phase equilibria, solid-state chemistry, surface phenomena, catalysis, and quantum chemistry.
- Explain the mechanisms and kinetics of complex chemical processes, including chain reactions, enzyme-catalyzed reactions, oscillatory reactions, and heterogeneous catalytic reactions.
- Apply thermodynamic and crystallographic principles to interpret phase behaviour, crystal structures, defects, and the physical properties of solid materials.
- Understand the relationship between surface properties, adsorption phenomena, and catalytic activity in chemical and industrial processes.
- Apply the principles of quantum mechanics to describe atomic and molecular structure, chemical bonding, spectroscopy, and electronic properties of matter.
- Develop analytical, mathematical, and problem-solving skills to interpret advanced concepts in physical chemistry and apply them to research and interdisciplinary scientific applications.

### Course Outcomes (COs)

After successful completion of the course, students will be able to:

- CO1:** Explain the mechanisms and kinetics of chain reactions, enzyme-catalyzed reactions, oscillatory reactions, and fast reactions using advanced kinetic models.
- CO2:** Apply Gibbs phase rule, Clausius–Clapeyron equation, and phase diagrams to analyze equilibrium behaviour in one- and two-component systems.
- CO3:** Interpret crystal structures using crystallographic principles, explain the role of defects and non-stoichiometry, and correlate structural features with the electrical, thermal, magnetic, and superconducting properties of solids.
- CO4:** Analyze adsorption phenomena, surface energetics, adsorption isotherms, and heterogeneous catalytic mechanisms, and evaluate their applications in chemical and industrial processes.
- CO5:** Apply the postulates of quantum mechanics, operator formalism, and approximate methods to solve problems related to atomic and molecular systems.
- CO6:** Explain molecular electronic structure using Molecular Orbital Theory, Valence Bond Theory, and Hückel Molecular Orbital Theory, and interpret bonding and electronic properties of molecules.

**Unit I Advanced Chemical Kinetics****Lecture Marks 10**

Chain reactions: General treatment and explanation of explosions; reaction mechanism and kinetics of  $\text{H}_2\text{-Br}_2$  reaction and pyrolysis of alkane.

Enzyme catalysis: Mechanism and kinetics of enzyme catalysis reaction

Oscillatory reactions: Mechanism and kinetics. Reactions in flow systems; kinetics of fast reactions.

**Unit II Phase Equilibria****Lecture Marks 10**

Concept of phases, components, and degrees of freedom; derivation of Gibbs Phase Rule for nonreactive and reactive systems; Clausius-Clapeyron equation and its applications to solid-liquid, liquid-vapour, and solid-vapour equilibria; Phase diagram of one-component systems (water and sulphur) and two-component systems (silver-lead and  $\text{KI-H}_2\text{O}$ )

**Unit III Advanced Solid State****Lecture Marks 15**

Types of solids; Order - spatial, orientational; Symmetry in crystals - primitive lattice vector - Wigner-Seitz cell - crystal systems - Bravais lattices - crystallographic point groups and space groups; X-ray diffraction - systematic absences - reciprocal lattice - Ewald construction - structure factor - crystal structure solution and refinement - common crystal structure motifs; quasicrystals. Point, line and plane defects; Intrinsic and extrinsic defects - vacancies, Schottky and Frenkel defects - charge compensation; Nonstoichiometry and defects - thermodynamic and structural aspects; Color centres. Lattice vibrations - phonon spectrum; Lattice heat capacity; Thermal expansion; Thermal conduction; Free electron theory - electrical conductivity and Ohm's law - Hall effect; Energy bands - band gap - metals and semiconductors - intrinsic and extrinsic semiconductors; Hopping semiconductors; p-n junctions; Semiconductor/metal transition; Superconductivity- Meissner effect- type I and II superconductors- isotope effect- basic concepts of BCS theory- manifestations of the energy gap- Josephson devices.

**Unit IV Surface Chemistry and Catalysis****Lecture Marks 15**

Adsorption: Physical adsorption, chemisorption, nature of the adsorbed state; thermodynamics of adsorption; factors affecting adsorption.

Adsorption from solution: surface tension and surface free energy, application of surface tension, capillary action: Young-Laplace equation; formation of bubbles: Kelvin equation. Capillary condensation; adsorption in micropores and hysteresis loop; Gibbs adsorption equation; surface active and surface inactive materials

Adsorption isotherms: Freundlich isotherm, Langmuir isotherm and BET isotherm; determination of the surface area of an adsorbent (Langmuir and BET equation); isosteric enthalpy of adsorption.

Catalytic activity at surfaces: mechanism of surface reaction; Langmuir-Hinshelwood and Eley-Rideal model; kinetic effects of surface heterogeneity and interactions. Kinetics of heterogeneous catalysis: unimolecular and bimolecular surface reactions.

**Unit V- Revision Quantum Chemistry****Lecture Marks 20**

Postulates of quantum mechanics, Operator algebra, Properties of hermitian operators, Eigenvalue problem, Commutators and Uncertainty Principle, Elementary applications of quantum mechanics- unbound motion in one dimension, Tunneling, Bound motion- particle-in-a-box (1D & 3D), harmonic oscillator and rigid rotor, Angular momentum algebra- Hydrogen atom, Methods of obtaining approximate solution to the time independent Schrödinger equation- perturbation theory and variational method, Application: Many electron atoms. Spin and Pauli exclusion principle, Hund's rule. Slater determinants, Electronic term symbols. Born- Oppenheimer approximation, LCAO-MO and VB treatment of the Hydrogen molecule and Hydrogen molecule ion, Comparison of Molecular Orbital and Valence Bond Methods. Huckel molecular orbital theory: Postulates, application to ethylene, butadiene, and benzene. Introduction to extended Huckel theory

**Suggested reading**

- Atkins, P. W.; de Paula, J.; Keeler, J., *Physical Chemistry*, 11th Ed., Oxford University Press, New Delhi (2018).
- Silbey, R. J.; Alberty, R. A.; Bawendi, M. G., *Physical Chemistry*, 4th Ed., Wiley India, New Delhi (2006).
- Levine, I. N., *Physical Chemistry*, 6th Ed. McGraw Hill Education, New Delhi (2011).
- Laidler, K. J., *Chemical Kinetics*, 3rd Ed., Pearson Education, New Delhi (2011).
- Kapoor, K. L., *A Textbook of Physical Chemistry: States of Matter and Ions in Solution*, Vol. I, 6th Ed., McGraw Hill Education India (2019).
- Puri, B. R.; Sharma, L. R.; Pathania, M. S., *Principles of Physical Chemistry*; 47th Ed, Vishal Publishing, New Delhi (2017).
- Adamson, A. W.; Gast, A. P., *Physical Chemistry of Surfaces*, 6th Ed, Wiley India, New Delhi (2011).
- Shaw, D. J., *Introduction to Colloid and Surface Chemistry*, 4th Ed, Butterworths Heinemann, Oxford (1992).
- Moudgil, H. K., *Textbook of Physical Chemistry*, PHI Learning, New Delhi (2010).
- Chandra, A. K., *Introductory Quantum Chemistry*, 4th Ed., McGraw Hill Education India, New Delhi (2017).
- Levine, I. N., *Quantum Chemistry*, 7th Ed., Pearson Education India, New Delhi (2016).
- McQuarrie, D. A., *Quantum Chemistry*, Viva Books, New Delhi (2016).
- Lewers, E. G., *Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics*, 2nd Ed., Springer, New York (2011). 5. Jensen, F., *Introduction to Computational Chemistry*, 3rd Ed., Wiley-Blackwell, New Jersey (2017).
- Sen, B. K., *Quantum Chemistry Including Spectroscopy*, 2nd Ed., Kalyani Publishers, New Delhi (2004).
- Atkins, P. W., Friedman R. S., *Molecular Quantum Mechanics*, 5th Ed., Oxford University Press, New Delhi (2012).
- Prasad, R. K., *Quantum Chemistry*, 4th Ed., New Age International Publishers, New Delhi (2010).

## Semester VII

|                              |                                                                   |
|------------------------------|-------------------------------------------------------------------|
| <i>NCrF level</i>            | 6.0                                                               |
| <i>Title of the Course</i>   | <i>Research Methodology in Natural Sciences</i>                   |
| <i>Course code</i>           | <i>CHEM-704</i>                                                   |
| <i>Paper credit</i>          | <i>04 (L 3 – T 1 - P 0)</i>                                       |
| <i>Total Contact Hours</i>   | <i>45 hours</i>                                                   |
| <i>Distribution of Marks</i> | <i>100 (End semester examination 70 + internal assessment 30)</i> |

### Course Objectives

After completing this course, students will be able to

- Understand the philosophy and importance of scientific research.
- Formulate research questions and testable hypotheses.
- Design experiments using appropriate scientific methods.
- Perform literature surveys using scientific databases.
- Apply statistical tools for data analysis and interpretation.
- Write scientific reports, research papers, dissertations and project proposals.
- Understand research ethics, plagiarism, intellectual property rights and publication ethics.

### Course Outcomes (COs)

Upon successful completion of the course, students will be able to

**CO1:** Explain the principles and philosophy of scientific research.

**CO2:** Identify research problems and formulate hypotheses.

**CO3:** Design scientific experiments using appropriate methodologies.

**CO4:** Analyze and interpret scientific data using statistical tools.

**CO5:** Prepare scientific manuscripts, dissertations and research proposals.

**CO6:** Demonstrate ethical conduct in research and scientific publication.

### UNIT I: Foundations of Scientific Research

**(8 Hours)**

Nature and philosophy of scientific research: Definition, objectives, significance, characteristics, scientific thinking, scientific temper.

Types of research: Basic research, applied research, translational research, interdisciplinary research, multidisciplinary research, qualitative research, quantitative research.

Scientific method: Observation, problem identification, hypothesis, experimentation, data collection, analysis, interpretation, conclusion, theory development.

Research problem: Identification, selection, feasibility, scope, novelty, significance, research gap.

Research hypothesis: Definition, characteristics, formulation, null hypothesis, alternative hypothesis, hypothesis testing.

Variables in research: Independent variable, dependent variable, controlled variable, confounding variable, operational definition.

Research design: Exploratory research, descriptive research, analytical research, experimental research, survey research.

Reliability and validity: Internal validity, external validity, reliability, reproducibility, repeatability.

## **UNIT II: Literature Survey and Research Planning (8 Hours)**

Scientific literature: Primary literature, secondary literature, tertiary literature, review articles, books, monographs, conference proceedings, technical reports, patents.

Literature search: Keywords, Boolean operators, search strategies, advanced search techniques.

Scientific databases: Google Scholar, Scopus, Web of Science, ScienceDirect, PubMed, SpringerLink, Wiley Online Library, ACS Publications.

Bibliographic tools: Mendeley, Zotero, EndNote, citation management, reference organization.

Citation metrics: Citation index, impact factor, h-index, i10-index, journal ranking, quartile ranking.

Literature review: Critical analysis, synthesis of literature, identification of research gaps, conceptual framework.

Research proposal: Title, objectives, hypothesis, methodology, work plan, expected outcomes, budget estimation, timeline.

## **UNIT III: Experimental Design and Data Collection (8 Hours)**

Experimental design: Objectives, variables, controls, replication, randomization, blocking.

Sampling techniques: Random sampling, systematic sampling, stratified sampling, cluster sampling, purposive sampling.

Sample size: Statistical considerations, confidence level, power of study.

Laboratory practices: Good Laboratory Practices (GLP), laboratory notebook, documentation, record keeping.

Measurement: Accuracy, precision, sensitivity, selectivity, uncertainty, calibration, validation.

Experimental errors: Systematic errors, random errors, gross errors, error minimization.

Quality assurance: Quality control, standard operating procedures (SOP), validation protocols.

Data collection: Experimental observations, instrumental measurements, field observations, questionnaires, surveys.

## **UNIT IV: Statistical Methods in Scientific Research (8 Hours)**

Data classification: Qualitative data, quantitative data, discrete data, continuous data.

Descriptive statistics: Mean, median, mode, range, variance, standard deviation, coefficient of variation.

Probability concepts: Probability distribution, normal distribution, binomial distribution, Poisson distribution.

Statistical inference: Confidence interval, confidence level, sampling distribution.

Hypothesis testing: Null hypothesis, alternative hypothesis, p-value, significance level, Type I error, Type II error.

Statistical tests: Student's t-test, paired t-test, Chi-square test, F-test, one-way ANOVA.

Correlation and regression: Pearson correlation, Spearman correlation, linear regression, coefficient of determination.

Data visualization: Tables, graphs, histograms, scatter plots, bar charts, line graphs, box plots.

Software applications: MS Excel, R software, SPSS, Origin, GraphPad Prism.

#### **UNIT V: Scientific Writing and Publication (7 Hours)**

Scientific communication: Research paper, review article, technical report, thesis, dissertation, project report.

Research paper structure: Title, abstract, keywords, introduction, materials and methods, results, discussion, conclusion, references.

Scientific writing: Clarity, precision, objectivity, logical organization, technical language.

Tables and figures: Preparation, formatting, captions, graphical presentation, image quality.

Referencing styles: APA, MLA, Chicago, ACS, IEEE, Vancouver.

Scientific journals: Journal selection, indexing, open-access journals, subscription journals, predatory journals.

Publication process: Manuscript submission, editorial screening, peer review, revision, acceptance, publication.

Research communication: Oral presentation, poster presentation, seminar presentation, conference participation.

Research identifiers: DOI, ORCID, ResearcherID, Scopus Author ID.

#### **UNIT VI: Research Ethics and Intellectual Property Rights (6 Hours)**

Research ethics: Principles, integrity, accountability, transparency, responsible conduct of research.

Scientific misconduct: Fabrication, falsification, plagiarism, duplicate publication, salami publication, data manipulation.

Authorship ethics: Authorship criteria, corresponding author, acknowledgements, contributorship.

Conflict of interest: Financial conflict, academic conflict, disclosure policy.

Plagiarism: Types, detection methods, plagiarism checking software, prevention strategies.

Intellectual Property Rights (IPR): Copyright, patent, trademark, industrial design, geographical indication, trade secret.

Patent system: Patentability, patent application, patent filing, patent search, patent examination.

Technology transfer: Innovation, commercialization, licensing, entrepreneurship, startup ecosystem.

Research safety: Laboratory safety, biosafety, chemical safety, waste management, environmental safety.

Research governance: Institutional Ethics Committee (IEC), Institutional Animal Ethics Committee (IAEC), Institutional Biosafety Committee (IBSC), Human Ethics Committee, regulatory guidelines.

### **Practical / Tutorial Component**

- Literature survey using Google Scholar and Scopus.
- Searching scientific journals and patents.
- Using Mendeley/Zotero for reference management.
- Preparation of a research proposal.
- Scientific paper review and presentation.
- Statistical analysis using MS Excel/R.
- Graph plotting and regression analysis.
- Detection of plagiarism using plagiarism-checking software.
- Preparation of a scientific poster.
- Oral seminar presentation.
- Writing a research article in IMRAD format.
- Preparation of a dissertation synopsis.

### ***Suggested readings***

- Kothari, C. R., & Garg, G. (2019). *Research Methodology: Methods and Techniques* (4th ed.). New Age International Publishers.
- Soumitro Banerjee (2021), *Research Methodology for Natural Sciences*, IISc Press / World Scientific
- Creswell, J. W., & Creswell, J. D. (2023). *Research Design: Qualitative, Quantitative, and Mixed Methods Approaches* (7th ed.). Sage Publications.
- Miller, J. N., & Miller, J. C. (2018). *Statistics and Chemometrics for Analytical Chemistry* (7th ed.). Pearson.
- Alley, M. (2018). *The Craft of Scientific Writing* (4th ed.). Springer.

**N.B. Student can take similar MOOCs course available online in NPTEL/SWAYAM  
<https://nptel.ac.in/courses/127106227>**



## Semester VII

|                              |                                                            |
|------------------------------|------------------------------------------------------------|
| <i>NCrF level</i>            | 6.0                                                        |
| <i>Title of the Course</i>   | <i>Advanced Practical I</i>                                |
| <i>Course code</i>           | CHMM-705                                                   |
| <i>Paper credit</i>          | 02 (L 0 – T 0 - P 2)                                       |
| <i>Total Contact Hours</i>   | 60 hours                                                   |
| <i>Distribution of Marks</i> | 100 (End semester examination 70 + internal assessment 30) |

### **Course Objectives**

After successful completion of this course, students will be able to:

- Develop practical skills in the physicochemical and analytical characterization of environmental samples using standard analytical methods.
- Synthesize environmentally benign nanomaterials and functional materials using green chemistry principles and evaluate their applications.
- Perform laboratory experiments related to materials chemistry, nanotechnology, and environmental remediation using modern experimental techniques.
- Interpret experimental observations, analyze laboratory data, and prepare scientific reports following good laboratory practices.
- Develop problem-solving abilities, laboratory ethics, teamwork, and scientific communication skills required for research and industrial laboratories.

### **Course Outcomes (COs)**

Upon successful completion of this course, students will be able to:

- CO1:** Perform physicochemical and analytical investigations of environmental samples using standard laboratory methods and interpret the results with reference to national and international standards.
- CO2:** Synthesize nanomaterials, biodegradable polymers, conducting polymers, and coordination compounds using conventional and green chemistry approaches and evaluate their physicochemical properties.
- CO3:** Apply spectroscopic, electrochemical, adsorption, and magnetic characterization techniques for the analysis of advanced materials and environmental samples.
- CO4:** Analyze experimental data, interpret scientific observations, and prepare laboratory reports using appropriate analytical and statistical methods while adhering to Good Laboratory Practices (GLP).
- CO5:** Demonstrate professional competence in laboratory safety, green chemistry principles, teamwork, ethical scientific practices, and effective scientific communication required for multidisciplinary research and industrial applications.

### **Unit I Environmental and Analytical Chemistry (20 Hours)**

Students shall perform **any two** experiments.

- Physicochemical analysis of drinking water according to WHO/BIS standards: determination of pH, electrical conductivity, total dissolved solids (TDS), dissolved oxygen (DO), biochemical oxygen demand (BOD), chemical oxygen demand (COD), total hardness, chloride, nitrate, and fluoride.

- Estimation of heavy metals in water or soil samples using UV–Visible spectrophotometry or colorimetric methods.
- Determination of phosphate and nitrate in natural water samples.
- Extraction and identification of microplastics from environmental water samples.
- Preparation of activated carbon from agricultural waste and evaluation of its adsorption efficiency for organic dyes.

**Unit II: Green Chemistry and Sustainable Technologies (20 Hours)**

Students shall perform **any two** experiments.

- Green synthesis and characterization of silver nanoparticles using plant extracts.
- Eco-friendly synthesis and characterization of ZnO nanoparticles.
- Catalytic degradation of organic dyes using synthesized nanoparticles.
- Preparation and characterization of biodiesel from waste cooking oil.
- Preparation and characterization of biodegradable polymer films using starch or chitosan.

**UNIT III: Materials Chemistry and Nanotechnology (20 Hours)**

Students shall perform **any two** experiments.

- Preparation and characterization of conducting polymers (Polyaniline or Polypyrrole).
- Sol–gel synthesis and characterization of silica nanoparticles.
- Fabrication of thin films using dip-coating or spin-coating techniques.
- Preparation and electrochemical characterization of supercapacitor electrode materials.
- Synthesis and characterization of coordination compounds and determination of magnetic susceptibility.

**Suggested Readings**

1. A. K. De, *Environmental Chemistry*, New Age International Publishers.
2. D. A. Skoog, F. J. Holler and S. R. Crouch, *Principles of Instrumental Analysis*, Cengage Learning.
3. P. T. Anastas and J. C. Warner, *Green Chemistry: Theory and Practice*, Oxford University Press.
4. C. N. R. Rao, A. Müller and A. K. Cheetham (Eds.), *The Chemistry of Nanomaterials*, Wiley-VCH.
5. J. B. Yadav, *Advanced Practical Physical Chemistry*, Goel Publishing House.

**Suggested Assessment Pattern**
**Total Marks: 100**

| Internal Assessment (30 Marks)               |           | End-Semester Practical Examination (70 Marks)     |           |
|----------------------------------------------|-----------|---------------------------------------------------|-----------|
| Component                                    | Marks     | Component                                         | Marks     |
| Continuous laboratory performance            | 10        | Practical experiment (one experiment)             | 25x2=50   |
| Laboratory notebook/record                   | 10        | Observation, calculations and data interpretation | 10        |
| Internal viva-voce and laboratory discipline | 10        | Viva-voce                                         | 10        |
| <b>Total</b>                                 | <b>30</b> | <b>Total</b>                                      | <b>70</b> |

## Semester VIII

|                              |                                                            |
|------------------------------|------------------------------------------------------------|
| <i>NCrF level</i>            | 6.0                                                        |
| <i>Title of the Course</i>   | <i>Advanced Inorganic Chemistry - II</i>                   |
| <i>Course code</i>           | <i>CHEM-801</i>                                            |
| <i>Paper credit</i>          | 04 (L 4 – T 0 - P 0)                                       |
| <i>Total Contact Hours</i>   | 70 hours                                                   |
| <i>Distribution of Marks</i> | 100 (End semester examination 70 + internal assessment 30) |

### Course Objectives

Upon successful completion of this course, students will be able to:

- Develop an advanced understanding of organometallic compounds, bioinorganic systems, inorganic solids, cluster chemistry, inorganic polymers, and the applications of group theory in inorganic chemistry.
- Explain the synthesis, bonding, structure, reactivity, and applications of metal carbenes, metallocenes, inorganic clusters, boranes, and inorganic polymers using modern bonding theories.
- Understand the structural and functional roles of metal ions and metalloenzymes in important biological processes and their significance in bioinorganic chemistry.
- Apply crystallographic principles to interpret the structures and properties of important ionic solids and correlate lattice energy with their physical and chemical behaviour.
- Apply group theoretical concepts to predict molecular symmetry, construct molecular orbitals, interpret spectroscopic transitions, and analyze chemical bonding in polyatomic molecules and coordination compounds.
- Develop analytical and problem-solving skills for interpreting structural, spectroscopic, and bonding aspects of advanced inorganic compounds relevant to research and industrial applications.

### Course Outcomes (COs)

After successful completion of the course, students will be able to:

- CO1:** Explain the synthesis, structure, bonding, reactivity, and applications of metal carbenes, carbynes, Tebbe's reagent, ferrocene, and other metallocenes using modern organometallic concepts.
- CO2:** Describe the structure, catalytic functions, and reaction mechanisms of biologically important metalloenzymes and metalloproteins involved in photosynthesis, nitrogen fixation, oxidation–reduction reactions, and vitamin B<sub>12</sub>-dependent processes.
- CO3:** Explain the crystal structures of important ionic solids, evaluate the significance of lattice enthalpy, and correlate crystal structure with material properties.
- CO4:** Analyze the structure, bonding, electron counting, synthesis, and reactivity of metal carbonyl clusters, boranes, carboranes, metalloboranes, and Zintl ions using Wade's rules and isolobal analogy.

**CO5:** Explain the classification, synthesis, bonding, structure, and applications of inorganic polymers, including sulphur–nitrogen compounds, siloxanes, silicates, aluminosilicates, zeolites, and clays.

**CO6:** Apply group theoretical methods, including direct product representations, projection operators, and symmetry-adapted linear combinations (SALCs), to analyze molecular symmetry and chemical bonding.

**CO7:** Construct molecular orbital diagrams for polyatomic molecules and coordination compounds, predict spectroscopic selection rules, hybridization patterns, and electronic structures using group theory.

### **Unit I Advanced Organometallic chemistry**

**Lecture/Marks: 15**

Metal carbenes: Introduction to metal-carbon multiple bonds, classifications, Fischer carbene, Schrock carbene, (Synthesis, Structure, bonding, synthesis and application), Tebb's reagent, metal carbynes

Ferrocene: Preparation and reactions (acetylation, alkylation, nitration and halogenation, metallation, Mannich condensation). Structure and aromaticity, Comparison of aromaticity and reactivity with that of benzene, other metallocenes

### **Unit II Advanced Bioinorganic Chemistry**

**Lecture/Marks: 10**

Photosynthesis: reaction pathway, role of magnesium ions

Active site structure and activity of nitrogenase enzyme, xanthine oxidase, alcohol dehydrogenase, aldehyde oxidase, aldehyde dehydrogenase and V-B<sub>12</sub>

### **Unit III Inorganic solids**

**Lecture/Marks: 10**

Characteristic structure types of ionic solids: CsCl, NaCl, Spalerite and Wurtzite types of ZnS, fluorite and anti-fluorite, nickel arsenide, CdCl<sub>2</sub>, CdI<sub>2</sub>, rutile, perovskite and spinels, Lattice enthalpy, consequences of lattice enthalpy

### **Unit IV: Inorganic cluster, cage and polymer**

**Lecture/Marks: 15**

Metal carbonyl clusters (low and high nuclearity clusters), calculation of metal-metal bond, electron counting in carbonyl clusters, binuclear clusters containing metal-metal multiple bonds, Metal-metal quadruple bond in [Re<sub>2</sub>Cl<sub>8</sub>]<sup>2-</sup>, isolobal analogy, zintl ions, synthesis of carbonyl clusters

Structure and bonding in polyhedral boranes, carboranes, metalloboranes and metallocarboranes, styx notation; Wade's rule; electron count in polyhedral boranes; synthesis of polyhedral boranes.

Types of inorganic polymers, comparison with organic polymers, Synthesis, structure and bonding in sulphur-nitrogen compounds, siloxanes, iso- and hetero-poly anions, Structure and chemistry of silicates, aluminosilicates, zeolites and clays

### **Unit IV Applications of Group Theory**

**Lecture/Marks: 20**

Direct product representation, projection operator and symmetry-adapted linear combination (SALC), symmetry selection rules for IR, Raman and electronic spectra. Hybrid orbital and hybridisation in polyatomic molecules, construction of hybrid orbitals for sigma & π-bonding (e.g. D<sub>3h</sub>, D<sub>4h</sub>, T<sub>d</sub>,

Oh). Molecular Orbital Theory: LCAO-MO approach; Construction of MO diagrams of polyatomic molecules (e.g. BeH<sub>2</sub>, H<sub>2</sub>O, BH<sub>3</sub>, NH<sub>3</sub>, CH<sub>4</sub>) including coordination complexes (Oh and Td).

### Suggested reading

- F. A. Cotton, G. Wilkinson, C. A. Murillo & M. Bochmann, *Advanced Inorganic Chemistry*, 6th Edition, Wiley.
- J. E. Huheey, E. A. Keiter & R. L. Keiter, *Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson.
- Miessler, Fischer & Tarr, *Inorganic Chemistry*, 5th Edition, Pearson.
- Gary L. Miessler, Paul J. Fischer & Donald A. Tarr, *Inorganic Chemistry*, Pearson.
- Shriver, D. F., Weller, M., Overton, T., Rourke, J. & Armstrong, F., *Inorganic Chemistry*, Oxford University Press.
- Satya Prakash, G. D. Tuli, S. K. Basu & R. D. Madan, *Advanced Inorganic Chemistry*, S. Chand.
- P. L. Soni & Mohan Katyal, *Textbook of Inorganic Chemistry*, Sultan Chand & Sons.
- R. L. Dutta, *Inorganic Chemistry*, Part I & II, New Age International.
- Gurdeep Raj, *Advanced Inorganic Chemistry*, Goel Publishing House.
- B. R. Puri, L. R. Sharma & K. C. Kalia, *Principles of Inorganic Chemistry*, Vishal Publishing Co.
- A. K. De, *A Textbook of Inorganic Chemistry*, New Age International.

## Semester VIII

|                              |                                                            |
|------------------------------|------------------------------------------------------------|
| <i>NCrF level</i>            | 6.0                                                        |
| <i>Title of the Course</i>   | <i>Advanced Organic Chemistry - II</i>                     |
| <i>Course code</i>           | CHMM-802                                                   |
| <i>Paper credit</i>          | 04 (L 4 – T 0 - P 0)                                       |
| <i>Total Contact Hours</i>   | 70 hours                                                   |
| <i>Distribution of Marks</i> | 100 (End semester examination 70 + internal assessment 30) |

### Course Objectives

Upon successful completion of this course, students will be able to:

1. Develop an advanced understanding of organic photochemical and pericyclic reactions, including their mechanisms, stereochemical outcomes, and synthetic applications.
2. Explain the synthesis, structure, reactivity, and aromaticity of important heterocyclic compounds and correlate their chemical behaviour with electronic structure.
3. Analyze conformational and stereochemical aspects of organic molecules using modern stereochemical principles and chiroptical methods.
4. Apply contemporary synthetic methodologies involving organometallic reagents, selective reagents, and catalytic processes for efficient carbon–carbon and carbon–heteroatom bond formation.
5. Develop mechanistic reasoning and retrosynthetic skills for designing efficient synthetic routes to complex organic molecules.
6. Strengthen analytical and problem-solving abilities for interpreting reaction mechanisms, stereochemical behaviour, and modern synthetic transformations relevant to pharmaceutical, medicinal, and industrial chemistry.

### Course Outcomes (COs)

After successful completion of the course, students will be able to:

- CO1:** Explain the principles, mechanisms, and synthetic applications of organic photochemical and pericyclic reactions, including orbital symmetry and stereochemical selection rules.
- CO2:** Analyze the synthesis, aromaticity, electronic properties, and chemical reactivity of saturated and aromatic heterocyclic compounds, including fused and diazine systems.
- CO3:** Interpret conformational preferences, stereochemical effects, and chiroptical properties of organic molecules and correlate molecular structure with chemical reactivity.
- CO4:** Apply modern synthetic methodologies involving organopalladium coupling reactions, olefination reactions, and organometallic reagents for selective carbon–carbon bond formation.
- CO5:** Explain the role and synthetic applications of organosulphur compounds, enamines, hydroboration, organosilicon, organozinc, organocopper, and other selective reagents in advanced organic synthesis.
- CO6:** Predict reaction pathways, stereochemical outcomes, and product formation based on mechanistic principles and reagent selectivity.
- CO7:** Design efficient synthetic strategies using modern reagents, catalytic transformations, and retrosynthetic analysis for the synthesis of complex organic molecules.

**Unit I Organic Photochemistry and Pericyclic Reactions****Lecture Marks 20**

Introduction to organic photochemistry, electronic transitions, Laws of photochemistry, quantum yield; cis-trans isomerisation, Norrish Type I & II reactions, photoreduction of ketones, Paterno-Buchi reaction, Lumketone rearrangement, Di- $\pi$ -methane and Di- $\pi$ -methane type rearrangement, Aza-Di- $\pi$ -methane type rearrangement, rearrangement of dienones and  $\beta,\gamma$ -unsaturated ketones.

Introduction; types of pericyclic reactions: electrocyclic reactions, cycloaddition, 1,3-dipolar addition, cheletropic reactions, sigmatropic and group transfer reactions; Ene reaction; selection rules; general orbital symmetry rules.

**Unit II Advanced Heterocyclic Chemistry****Lecture Marks 15**

Syntheses of aziranes, oxiranes & thiiranes; ring openings and heteroatom extrusion; synthesis & reactions of azetidines, oxetanes & thietanes. Aromatic heterocycles: Synthesis and reactions of furan, thiophene, pyrrole, pyridine, quinoline, isoquinoline and indole. Concept of  $\pi$ -excessive and  $\pi$ -deficient heterocyclics. Condensed Five-membered Rings (1 Heteroatom): Synthesis and reactions of indole, benzofuran and benzothiophene. Diazines: Structural & chemical properties; Synthesis of pyridazines, pyrimidines, pyrazines, nucleophilic and electrophilic substitutions.

**Unit III Advanced Stereochemistry****Lecture Marks 15**

Conformational analysis of disubstituted cyclohexanes, cyclohexene, cyclohexanone, 2-alkyl, 3-alkyl, and 4-alkyl ketone effects. A 1,2 and A 1,3 strains. Conformation of fused systems - decalins and perhydrophenanthrenes. Effects of conformation on reactivity and mechanism of basic organic reactions of 6-membered ring compounds. Chiroptical properties - Optical rotatory dispersion, circular birefringence, circular dichroism, axial haloketone rule, octane rule.

**Unit IV Advanced Organic Synthesis****Lecture Marks 20**

Organometallic reagents in formation of carbon-carbon bonds: Organopalladium in C-C formation (Heck reaction, Stille, Suzuki, Sonogashira and Negishi Coupling). Formation of C=C bonds by elimination reactions, syn elimination; Wittig and related reactions, McMurry reaction, Peterson olefination, Julia reaction and Tebbe olefination. Use of organosulphur compounds for reversal of polarity (Corey-Seebach Umpolung). Allylic activation by  $\pi$ -allyl Ni and  $\pi$ -allyl Pd complexes. Application of Enamines, Hydroboration and trialkylsilyl halides in organic synthesis. Use of the following reagents: Organotin (TBTH), Lithium Diisopropyl Amide (LDA), Dicyclohexylcarbodiimide, Dicyanodichloroquinone (DDQ), Dimethyl dioxirane (DDO), lipase and other reagents of organozinc and organocopper.

**Suggested reading**

- Smith, M. B.; March, J., *March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure*, 7th Ed., Wiley India, New Delhi (2015).
- Nasipuri, D. *Stereochemistry of Organic Compounds: Principles and Applications*, 3rd Ed., New Age International Publishers, New Delhi (2018).
- Sengupta, S., *Basic Stereochemistry of Organic Molecules*, 2nd Ed., Oxford University Press, New Delhi (2018).
- Kalsi, P. S., *Stereochemistry: Conformation and Mechanism*, 10th Ed., New Age International Publishers, New Delhi (2019).

## Semester VIII

|                              |                                                                   |
|------------------------------|-------------------------------------------------------------------|
| <i>NCrF level</i>            | 6.0                                                               |
| <i>Title of the Course</i>   | <i>Advanced Physical Chemistry II</i>                             |
| <i>Course code</i>           | <i>CHMM-803</i>                                                   |
| <i>Paper credit</i>          | <i>04 (L 4 – T 0 - P 0)</i>                                       |
| <i>Total Contact Hours</i>   | <i>70 hours</i>                                                   |
| <i>Distribution of Marks</i> | <i>100 (End semester examination 70 + internal assessment 30)</i> |

### Course Objectives

Upon successful completion of this course, students will be able to:

- Develop an advanced understanding of chemical kinetics, thermodynamics, phase equilibria, and polymer chemistry through quantitative and molecular-level approaches.
- Explain the theories of reaction rates, reaction mechanisms, solvent effects, and the factors governing the kinetics of homogeneous reactions.
- Apply thermodynamic principles to describe non-ideal systems, phase transitions, partial molar properties, and chemical equilibria.
- Interpret phase diagrams of binary and ternary systems and apply distribution laws to extraction and separation processes.
- Understand the structure, molecular characteristics, polymerization mechanisms, and physicochemical behaviour of macromolecules.
- Develop analytical, mathematical, and problem-solving skills to explain physicochemical phenomena and apply them in research, industrial chemistry, and materials science.

### Course Outcomes (COs)

After successful completion of the course, students will be able to:

- CO1:** Explain the principles of kinetic and thermodynamic control of reactions and evaluate reaction mechanisms using collision theory, transition state theory, and unimolecular reaction models.
- CO2:** Analyze the influence of solvent, ionic strength, dielectric constant, and diffusion on reaction rates and predict kinetic behaviour in solution-phase reactions.
- CO3:** Apply the concepts of fugacity, activity, chemical potential, Gibbs–Duhem equation, and partial molar properties to interpret the thermodynamic behaviour of ideal and non-ideal systems.
- CO4:** Interpret binary and ternary phase diagrams, explain eutectic and congruent/incongruent melting systems, and apply the Nernst distribution law to solvent extraction and related separation processes.
- CO5:** Explain the classification, molecular characteristics, polymerization mechanisms, and molecular weight determination methods of polymers and macromolecules.
- CO6:** Analyze the configuration, conformation, diffusion behaviour, and chain statistics of polymer molecules using appropriate theoretical models.



**Unit-I Chemical Kinetics III****Lecture Marks 15**

Kinetic control and thermodynamic control of reaction, Theories of reaction rate: Arrhenius theory; simple collision theory (SCT); steric factor, activated complex theory (ACT); thermodynamics of reaction rate and entropy of activation. Theories of unimolecular reactions: Lindemann mechanism and Hinshelwood treatment.

Reaction in solution: diffusion-controlled and chemically controlled reaction; factors affecting reaction rate in solution; effect of solvent and ionic strength on the rate constant: primary and secondary salt effect; effect of the dielectric constant of the medium on the rate of reaction in solution.

**Unit II Chemical Thermodynamics III****Lecture/Marks: 15**

Fugacity and activity and their variation with temperature and pressure, Graphical method for the determination of fugacity; fugacity of van der Waals gases

Partial molar quantities and their physical significance; Partial molar free energy (chemical potential) and its variation with temperature and pressure; Gibbs-Duhem equation

Gibbs free energy and entropy of mixing of ideal gases; partial molar volumes; method of determination of partial molar volumes, Thermodynamic description of phase transitions and Clapeyron-Clausius equation

**Unit III Phase Equilibria-II****Lecture/Marks: 15**

Phase diagrams for systems of solid-liquid equilibria involving eutectic, congruent and incongruent melting points, solid solutions. Three-component systems, water-chloroform-acetic acid system, triangular plots

Nernst distribution law and its limitations, thermodynamic derivation, Modification of distribution law to cases of association and dissociation of solute and complex formation, Application of the law in the process of extraction

**Unit IV Macromolecules****Lecture Marks: 15**

Brief overview of polymers: Classification and types of polymers. Concept and types of molecular weight; distribution of molecular weight in polymers; significance of molecular weight; degree of polymerization and chain length, Methods of determining molecular weights of macromolecules: End group analysis; osmometry, viscometry and light scattering methods. Types of polymerization; kinetics of addition and step growth (condensation) polymerisation, Different models for describing the size and shape of dissolved macromolecules; configuration and conformation of macromolecules, Diffusion and Stokes-Einstein equation, Distribution of chain lengths: average end-to-end, root mean square end-to-end and most probable end-to-end chain length.

**Suggested reading**

- Atkins, P. W.; de Paula, J.; Keeler, J., *Physical Chemistry*, 11th Ed., Oxford University Press, New Delhi (2018).

- Silbey, R. J.; Alberty, R. A.; Bawendi, M. G., *Physical Chemistry*, 4th Ed., Wiley India, New Delhi (2006).
- Levine, I. N., *Physical Chemistry*, 6th Ed. McGraw Hill Education, New Delhi (2011).
- Laidler, K. J., *Chemical Kinetics*, 3rd Ed., Pearson Education, New Delhi (2011).
- Kapoor, K. L., *A Textbook of Physical Chemistry: States of Matter and Ions in Solution*, Vol. I, 6th Ed., McGraw Hill Education India (2019).
- Puri, B. R.; Sharma, L. R.; Pathania, M. S., *Principles of Physical Chemistry*; 47th Ed, Vishal Publishing, New Delhi (2017).
- Kapoor, K. L., *A Textbook of Physical Chemistry: Thermodynamics and Chemical Equilibrium*, Vol. II, 6th Ed., McGraw Hill Education India (2019).
- Prigogine, I., *Introduction to Thermodynamics of Irreversible Processes*, 3rd Ed., Wiley (1968).
- Billmeyer, F. W., *Textbook of Polymer Science*, 3rd Ed., Wiley India, New Delhi (2007).
- Gowariker, V. R., Viswanathan, N. V. and Sreedhar, J., *Polymer Science*, 3rd Ed., New Age International Publishers, New Delhi (2019).

## Semester VIII

|                              |                                                                    |
|------------------------------|--------------------------------------------------------------------|
| <i>NCrF level</i>            | 6.0                                                                |
| <i>Title of the Course</i>   | <i>Advanced Chemistry Practical II</i>                             |
| <i>Course code</i>           | <i>CHMM-804</i>                                                    |
| <i>Paper credit</i>          | <i>08 (L 0 – T 2 - P 6)</i>                                        |
| <i>Total Contact Hours</i>   | <i>180 hours</i>                                                   |
| <i>Distribution of Marks</i> | <i>200 (End semester examination 140 + internal assessment 60)</i> |

### Course Objectives

After successful completion of this course, students will be able to:

- Perform advanced inorganic, organic and physical chemistry experiments independently.
- Synthesize and characterize coordination compounds, nanomaterials and organic molecules.
- Apply modern instrumental techniques such as UV–Visible spectroscopy, FTIR and TLC for qualitative and quantitative analysis.
- Analyse experimental data using statistical and computational tools.
- Interpret spectroscopic and kinetic data and prepare scientific laboratory reports.
- Demonstrate safe laboratory practices, research ethics and scientific communication skills.

### Course Outcomes (COs)

Upon successful completion of the course, students will be able to:

- CO1:** Demonstrate proficiency in advanced laboratory techniques for inorganic, organic, and physical chemistry, including quantitative analysis, synthesis of coordination compounds, organic synthesis, kinetic studies, electrochemical measurements, and thermodynamic investigations.
- CO2:** Synthesize, purify, and characterize coordination compounds, nanomaterials, semiconductor materials, and organic compounds using appropriate experimental techniques and instrumental methods such as TLC, UV–Visible spectroscopy, FTIR spectroscopy, and other available analytical tools.
- CO3:** Analyze, interpret, and present experimental data using appropriate mathematical, statistical, and computational methods, including spreadsheet software (Excel/Origin/R), and apply scientific principles to solve chemical problems.
- CO4:** Apply research methodology, scientific literature survey, molecular visualization, laboratory safety practices, green chemistry principles, and good laboratory practices (GLP) in planning, executing, and documenting laboratory investigations.
- CO5:** Communicate scientific findings effectively through laboratory records, technical reports, research paper presentations, and oral discussions while demonstrating ethical conduct, teamwork, and professional competence required for research and industrial laboratories.

### **Part A Inorganic Chemistry Practical**

*Students shall perform any SIX experiments, including: One quantitative analysis, Three coordination/synthetic chemistry experiments, One nanomaterials or polyoxometallate experiment, One instrumental/computational experiment*

- Quantitative analysis (binary mixture, alloy, ore) - Ca-Mg ore, Cu-Zn alloy, Pb-Sn alloy, Ni in an alloy etc.
- Solution phase synthesis of coordination compounds e.g. vanadylacetylacetonate, potassium trisoxalatometal(III) trihydrate etc.; characterization, properties and applications (e.g. catalysis).
- Synthesis of coordination compounds through ligand synthesis and spectroscopic characterization, e.g. preparation of bis(*N,N*-disalicylideneethylenediamine)( $\mu$ -aquadicobalt(II)).
- Solid phase synthesis of coordination compounds (e.g. Reinecke salt, *trans*-bisglycinatocopper(II)) and their properties.
- Isomerism in coordination compounds. e.g. conversion of chloropentammine cobalt(III) chloride to nitro and nitroso isomers, *cis*- and *trans*-dichlorobis(ethylenediamine)cobalt(III) chloride etc.
- Preparation of metal(II) isonicotinatatetrahydrates, characterization, use as precursors to metal oxides.
- Synthesis of metal nanoparticles (Cu, Ag, Au, etc.), characterization and investigation of their optical properties.
- Synthesis and characterization of semiconductor nanocrystals (CdS, ZnS, ZnO etc.).
- Preparation of polyoxometallates (e.g. tetrabutylammoniumhexamolybdate(VI)), characterization.
- Quantitative determination of components in food (Fe, Zn, I, Ca, etc.)
- Applications of UV-Visible spectroscopy: (a) Verification of Beer-Lambert's law, (b) Determination of composition of Fe(III)-salicylate complex by Job's method, (c) Kinetic study of the acetone-iodine reaction by colorimetry.

### **Part B Organic Chemistry Practical**

*Students shall perform any SIX experiments including at least one qualitative analysis, one estimation experiment, three synthetic experiments and one instrumental characterization experiment.*

- Qualitative analysis : Binary mixture analysis (solid-solid, solid-liquid, liquid-liquid)
- Estimation of amino acids using titrimetric methods
- Estimation of sugars using titrimetric (redox) methods.
- Solvent free reductive amination: Synthesis of imine from aldehyde and amine in solvent free condition and its reduction to amine using NaBH<sub>4</sub>.
- Oxidation of phenanthrene to phenanthrene-dione and its subsequent condensation to imidazophenanthrene derivative.
- Organic preparations involving two or more steps: (a) Benzopinacolone from benzophenone via benzopinacol (b) Benzilic acid from benzoin (c) Dibenzyl from benzoin (d) Anthranilic acid from phthalic anhydride (e) Any halogenation reaction etc. 2. Greener practice in organic synthesis: (a) Acetylation of primary amine (b) Bromination of acetanilide (c) Nitration of phenol (d) Pinacol Pinacolone rearrangement
- Multicomponent reaction of aldehyde,  $\beta$ -keto ester and urea/thiourea for the synthesis of dihydro-pyrimidine derivatives (Biginelli reaction)
- Multicomponent reaction of aldehyde,  $\beta$ -keto ester and ammonia for the synthesis of dihydro-pyridine derivatives (Hantzsch Pyridine Synthesis)
- Extraction, purification and characterization of natural products (curcumin/caffeine/eugenol/limonene/chlorophyll) using TLC and UV-Visible spectroscopy.

Note: During all organic synthesis experiments, students shall monitor the progress of the reaction using Thin Layer Chromatography (TLC) with appropriate solvent systems and determination of R<sub>f</sub>

values. Synthesized compounds should be characterized, wherever applicable, using melting point determination, FTIR spectroscopy and UV–Visible spectroscopy.

### **Part C Physical Chemistry Practical**

*Students shall perform any SIX experiments covering chemical kinetics, electrochemistry, thermodynamics, surface chemistry and computer-assisted data analysis.*

- Determination of the temperature coefficient and activation energy of acid hydrolysis of methyl acetate using the least squares method.
- Study of the kinetics of saponification of ethyl acetate by sodium hydroxide and determination of the rate constant and reaction order.
- Kinetics of the reaction between iodine and acetone in acidic medium and determination of the reaction order.
- Investigation of the kinetics of oxidation of ethanol by chromium(VI) and determination of the rate constant.
- Determination of the equivalent conductivity of acetic acid at infinite dilution by Kohlrausch's law and calculation of its dissociation constant.
- Conductometric titration of binary mixtures:  $\text{HCl} + \text{CH}_3\text{COOH}$ ,  $\text{H}_2\text{SO}_4 + \text{CuSO}_4$ ,  $\text{HCl} + \text{KCl}$
- Potentiometric estimation of hydrochloric acid, acetic acid, and their binary mixture using standard sodium hydroxide.
- Potentiometric titration of ferrous ammonium sulphate with potassium dichromate and determination of the standard electrode potential of the  $\text{Fe}^{3+}/\text{Fe}^{2+}$  system.
- Adsorption of methylene blue on activated carbon and analysis using Langmuir and Freundlich adsorption isotherms.
- Determination of adsorption kinetics of dye on activated carbon.
- Determination of the critical micelle concentration (CMC) of a detergent by surface tension measurement.
- Determination of the heat capacity of a calorimeter and the enthalpy of solution of ammonium chloride.
- Determination of the Van't Hoff factor of an electrolyte by cryoscopic method.
- Determination of the solubility product of calcium hydroxide by studying its solubility in sodium hydroxide solution.
- Computer-assisted data analysis using least-squares fitting (linear and exponential plots) and determination of kinetic and thermodynamic parameters using spreadsheet software (Excel/Origin/R).

### **Tutorial Component (2 Credits)**

Students shall complete at least two of the following tutorial activities

- Literature survey using SciFinder, Reaxys, PubChem and Web of Science.
- Research paper presentation and discussion.
- Interpretation of UV–Visible, IR, NMR and Mass spectra.
- Statistical analysis of experimental data using Excel, Origin or R.
- Laboratory safety, GLP and chemical waste management.

- Scientific report writing and referencing.
- Introduction to computational chemistry and molecular visualization.

The Department may introduce additional experiments or modify existing experiments from time to time in accordance with advances in chemical sciences and the availability of laboratory facilities, with the approval of the Board of Studies.

### Books Recommended

- J. Mendham, R. C. Denney, J. D. Barnes, M. Thomas, B. Sivasankar, Vogel's Textbook of Quantitative Chemical Analysis, 6th Edition, Pearson, 2009.
- Furniss, B. S.; Hannaford, A. J.; Smith, P. W. G.; Tatchell, A. R., Vogel's Textbook of Practical Organic Chemistry, 5th Ed., Pearson Education India, New Delhi (2003).
- Mann, F. G.; Saunders, B. C., Practical Organic Chemistry, 4th Ed., Pearson Education India, New Delhi (2009).
- Clarke, H. T., A Handbook of Organic Analysis: Qualitative and Quantitative, 4th Ed., CBS Publishers, New Delhi (2007).
- J. B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 27th Edison, 2008.
- J. N. Gurtu and A. Gurtu, Advanced Physical Chemistry Experiments, PragatiPrakashan, 6th Edition, 2014.
- Other Sources: *Journal of Chemical Education*, ACS Publications.

### Assessment Pattern (Total Marks: 200)

| A. Continuous Internal Assessment                                         |           |           |           | (60 Marks)  |
|---------------------------------------------------------------------------|-----------|-----------|-----------|-------------|
| Component                                                                 | Inorganic | Organic   | Physical  | Total       |
| Continuous laboratory performance                                         | 10        | 10        | 10        | 30          |
| Laboratory record book                                                    | 5         | 5         | 5         | 15          |
| Viva during practical classes                                             | 5         | 5         | 5         | 15          |
| <b>Total</b>                                                              | <b>20</b> | <b>20</b> | <b>20</b> | <b>60</b>   |
| B. Tutorial Assessment                                                    |           |           |           | (40 Marks)  |
| Component                                                                 |           |           |           | Marks       |
| Literature survey/Scientific database search                              |           |           |           | 10          |
| Seminar/Research paper presentation                                       |           |           |           | 10          |
| Spectral interpretation/Computational exercise/Data analysis              |           |           |           | 10          |
| Scientific report writing/Assignment                                      |           |           |           | 10          |
| <b>Total</b>                                                              |           |           |           | <b>40</b>   |
| C. End Semester Practical Examination                                     |           |           |           | (100 Marks) |
| Each student performs <b>one experiment from each branch.</b>             |           |           |           |             |
| Component                                                                 |           |           |           | Marks       |
| Inorganic Chemistry Practical                                             |           |           |           | 25          |
| Organic Chemistry Practical                                               |           |           |           | 25          |
| Physical Chemistry Practical                                              |           |           |           | 25          |
| Comprehensive Viva-Voce (covering all three branches and tutorial topics) |           |           |           | 18          |
| Discipline/ team work/ cooperation                                        |           |           |           | 07          |
| <b>Total</b>                                                              |           |           |           | <b>100</b>  |

**End of the Syllabus**