

# CHEMISTRY CURRICULUM



B.Sc. (Hons.) Chemistry – 4 Years program
B.Sc. (Hons., with Research) Chemistry – 4 Years program
B.Sc. (Hons.) Chemistry (Specialization) – 4 Years program
B.Sc. (Hons., with Research) Chemistry (Specialization) – 4 Years program



DEPARTMENT OF CHEMISTRY PONDICHERRY UNIVERSITY 2023

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## **CREATIVE CHEMISTRY**

## **Chemistry Curriculum 2022**

An outcome of continued, collective, and collaborative effort with a vision to develop an innovative, responsive, inclusive, flexible, and dynamic curriculum in tune with the global educational needs for the 21<sup>st</sup> century and beyond

Our curricular structure, courses, pedagogy, and assessment has truly catered to the development of diversified, integrated, interdisciplinary knowledge and skills as well as inculcation of values to survive in the highly competitive knowledge and skilled society

"To boldly explore and set new chemical frontiers in the life sciences, physical sciences, medicine, energy, materials, and environmental sciences through visionary research, innovation, collaboration, and scholarship"

# **DEPARTMENT OF CHEMISTRY**

Department of Chemistry, Pondicherry University, since its inception is a leader and trendsetter in developing and implementing a relevant model curriculum which has been adapted by several premier institutes in India. Chemistry curriculum 2022, called Creative Chemistry, is an outcome of our continued, collective, and collaborative effort with a vision to develop an innovative, responsive, inclusive, flexible, and dynamic curriculum in tune with the global educational needs for the 21<sup>st</sup> century and the National Education Policy NEP 2020. Our curricular structure, courses, pedagogy, and assessment has genuinely catered to the development of diversified, integrated, interdisciplinary knowledge and skills as well as inculcated the values needed to survive in the highly competitive, skilled, and knowledge society.

## Vision and Mission

#### Vision

Chemists are driving a molecular revolution of unprecedented magnitude and impact, that will transform the whole of science and the world as we know it. Chemistry—the quintessential molecular science—is enabling us to "see and explore" with atomistic resolution, these previously unobservable scientific frontiers.

With this new knowledge, chemists have created remarkable new molecules, materials, tools, and theories for the benefit of Science and Society. We can now make, modify, simulate, and interrogate most molecules that have existed since time immemorial. Equally importantly, we can design, make, and study fascinating new ones.

Chemistry at Pondicherry University is a leader of the molecular revolution, addressing the most challenging and important questions in the physical and life sciences of the 21st century. By leveraging its multi-disciplinary vision, its culture of synergistic collaboration and translational science, and excellence in the physical, biological and engineering sciences, Chemistry at Pondicherry University is opening new vistas and frontiers and fundamentally new and innovative ways to address the increasingly complex scientific, health, energy and environmental needs of our present as well as futuristic times.

#### Mission

#### **Discover, Create and Understand**

Through independent research and synergistic collaborations with scientists and entrepreneurs around the world, the Department continues to build on its distinguished history of major advances in chemical science and computation, creating innovations that open new research opportunities in multiple domains of sciences.

#### **Inspire and Educate**

Through spirited mentoring of future researchers, innovative instruction of students within Chemistry and across majors, and creative approaches to scientific communication, visualization and computation, the Department trains and informs tomorrow's leading scientists, professionals, and policymakers, and fosters new knowledge of the chemistries underlying living systems and physical processes.

Inspiring and educating undergraduate students in chemistry and molecular- driven sciences in the core concepts of chemistry and scientific methods. Advancing a knowledge platform that supports an invent-and-design culture in graduate and undergraduate chemistry education, and empowers students to address and solve challenges of global significance.

Reaching out to our future thought leaders—students of all backgrounds from college to doctoral candidates—to share the power of chemistry to create new knowledge directed at the major unmet needs of our time.

Supporting and advancing worldwide community of chemistry scholars Informing the public about the excitement of science, its impact on everyday life, and the crucial role it plays in human health, energy, and environmental stewardship.

#### Lead and Collaborate

The Chemistry Department is blazing a path of excellence that will define the future of scholarship in the chemical sciences by supporting a creative environment that fosters discovery, learning and collaboration, and attracting the best faculty and students to the university.

## 1. Terms and Definitions

Terms used in the NEP- Regulations shall have the meaning assigned to them as given below unless the context otherwise requires.

- a. **"Credit**" is a unit by which the coursework is measured. It determines the number of hours of instruction required per week during a semester (Minimum 15 weeks). One credit is equivalent to 15 hours of teaching (lecture and /or tutorial) or 30 hours of practical and/or field work or community engagement and service per semester.
- b. "Academic Year" means the year starting in the month of June and ending in the succeeding month of May.
- c. "Semester" means 15-16 weeks of teaching-learning sessions of which two weeks shall be set apart for examination and evaluation; A semester comprises 90 working days and an academic year is divided into two semesters.
- d. **"Summer term"** is for 8 weeks during summer vacation. Internship/apprenticeship/work based vocational education and training can be carried out during the summer term, especially by students who wish to exit after two semesters or four semesters of study.
- e. "**Grade**" means a letter grade assigned to a student in a Course for her/his performance at academic sessions as denoted in symbols of: O(outstanding), A+(Excellent), A(Very good), B+(Good), B(Above average), C(Average), P(Pass) F(Fail) and Ab( Absent) with a numeric value of O=10, A+=9, A=8, B+=7, B=6, C=5 P=4, and F=0, Ab=0;
- f. **"Semester Grade Point Average (SGPA)**" is computed from the grades as a measure of the students' performance in a given semester.
- g. **"Cumulative GPA (CGPA)**" is the weighted average of all courses the student has taken in a given Programme;
- h. "**Programme**" means a set of Courses that allows a student to structure and study to attain the status of being admitted to a Degree/Diploma of the University;
- i. **"Programme Committee**" means an Academic Committee constituted by the University for the purpose of conducting an Academic Programme;
- j. "**Credit Requirement**" for a Degree/Diploma/Certificate Programme means the minimum number of credits that a student shall accumulate to achieve the status of being qualified to receive the said Degree, Diploma/Certificate as the case may be;
- k. **"Exit option**" means the option exercised by the students, to leave the Programme at the end of any given Academic year;
- 1. "**Lateral entry**" means a student being admitted into an ongoing Programme of the University other than in the 1st year of the programme.

## 2. Programs Offered

# 4 Years B.Sc. (Hons.) Chemistry/B.Sc. (Hons. with Research) Chemistry Programs

#### "A holistic integrated approach to appreciate CHEMISTRY AS CENTRAL SCIENCE"

#### **Program Features**

- An integrated approach to all sub-disciplines of chemistry
- 4-year/8-semester Program leading to B.Sc. (Hons.)/ B.Sc. (Hons. with Research) Chemistry certification
- Multiple specialization options for students to pursue their goal
- Student centric learning plans
- Advanced level theory courses aimed towards research inclinations
- One-year research project leading to undergraduate thesis submission
- Project based laboratory experiments to develop research skills
- Flexibility to choose pure chemistry or inter-disciplinary or cross-disciplinary curriculum

This program envisages to bring a transformative approach to undergraduate chemistry degree program. This program will provide an opportunity to students to acquire the necessary soft skills such as complex problem solving, critical thinking, creative thinking, oral and written communication skills. This program gives the opportunity to students to mix-and-match their learning plans to achieve their future goals in advanced studies or career development.

This four-year Program covers basic, foundation and advanced courses with special focus on pure chemistry such as: Analytical Chemistry, Inorganic Chemistry, Organic Chemistry, Biochemistry, Physical Chemistry, Computational Chemistry, Research Chemistry, Identification and Analysis of Organic compounds, Spectroscopy of Organic Compounds and Synthesis of Organic Compounds. Components such as summer internship, seminar participation, independent research and comprehensive viva are opportunities offered to students to get wide-ranging experiences in research and develop much needed career skills.

Laboratory courses are designed towards equipping the students with multiple skills to enable them to enter any career of their choice, say research, industry or academic arena. In addition, they develop skills in eco-friendly chemistry practices, organizing the work, maintaining a chemistry laboratory, safe laboratory practices, micro-scale experiments, and hands on experience with modern instruments. Students also learn through tutorial instructions from research scholars, post-doctorate researchers, and visiting experts. Laboratory courses also inculcate ethics, values, and competence in communication and collaboration culture.

The syllabi given in the following pages are guidelines for the tutors and the students. The course tutor(s) has the scope and responsibility to innovate and modernize the content to suit the need of the students and develop her/his own methods to evaluate various competencies. The course tutor(s) may liberally adopt interactive classroom scenarios and integrated online education management system and other ICT tools to impart knowledge. Assignments, quizzes, question-answer sessions, problem solving sessions, tutorials, written examinations are the

suggested general methods of instruction and evaluation. Students are expected to use library and internet facilities to augment classroom activities to build their knowledge.

Details of Program structure, syllabus for each course and recommended number of credits for every semester is given in the following pages. It is mandatory for every student to complete the credit requirements for the award of degree certificate. However, students have liberty to choose their semester workload as per their convenience and ability. The maximum period for completion of the Program shall be 12 semesters.

#### **Program Purpose**

The purpose of the four-years B.Sc. (Hons.)/ B.Sc. (Hons. with Research) Chemistry program at Pondicherry University is to develop an integrated approach to learning chemistry and appreciate and apply the acquired knowledge in solving societal, environmental and health issues of the world. The following objectives are expected to be attained

- Appreciate the necessity for an integrated approach through the spectacles of biology, chemistry, mathematics, and physics in learning science
- Appreciate and understand the underlying atomistic behavior of the chemical systems when exhibiting their properties
- Apply the basic knowledge in chemistry, mathematics, physics in understanding and predicting the properties and behavior of chemical systems
- Develop an attitude to view chemistry as the central science
- Train the students to approach chemistry as an integrated science instead of studying as a collection of several independent sub-domains of knowledge
- Develop experimental skill towards research career
- Develop skills to appreciate and understand concepts of chemistry in books and mind through experimental designs and simulations
- Develop skill towards using various software and digital technology to understand chemical properties
- Develop written and oral communication skill
- Develop competence on various aspects of scientific research and investigations

#### **Program Learning Outcomes**

Students will acquire a firm foundation in the fundamentals and application of current chemical and scientific theories including those in Analytical, Inorganic, Organic and Physical Chemistries. Majors with skills in extensive laboratory work and knowledge in various interdisciplinary sciences, are eligible to be certified by the American Chemical Society and/or Royal Chemical Society.

- Students can design and carry out scientific experiments as well as accurately record and analyze the results of such experiments.
- Students can develop skills in problem solving, critical thinking and analytical reasoning as applied to scientific problems.
- Students can develop ability to communicate the results of scientific work in oral, written, and electronic formats to both scientists and the public at large.

- Students will acquire skills to explore new areas of research in chemistry and allied fields of science and technology.
- Students will appreciate the central role of chemistry in our society and use this as a basis for ethical behavior in issues facing chemists, including an understanding of safe handling of chemicals, environmental issues and key issues facing our society in energy, health, medicine, and chemical industries.
- Students can explain why chemistry is an integral activity for addressing social, economic, and environmental problems.
- Students will function as members of an interdisciplinary problem-solving team.

#### **Career Opportunities**

Graduates of B.Sc. (Hons.)/ B.Sc. (Hons. with Research) Chemistry may pursue a career path in pharmaceuticals, food and beverage companies, cosmetics companies, oil and petroleum companies, mineral companies, and chemical manufacturing companies, and clinical facilities. They may apply as a process chemist, industrial chemist, agricultural chemist, analytical chemist, clinical biochemist, cosmetic chemist, chemical analyst, or a chemistry teacher or professor.

#### **Suggested Specialization Options**

Students enrolling for B.Sc. (Hons.)/ B.Sc. (Hons. with Research) Chemistry can earn credits from other disciplines to construct their learning plans leading to specialization. Students shall enroll for not less than 32 credits under minor-discipline credits for this purpose in which a minimum of 12 credits from respective specialization subject)

The following is an illustration of few popular specialization combinations

- Chemical Biology
- Medicinal Chemistry
- Chemical Physics
- Environmental Chemistry
- Food Chemistry
- Computational Chemistry
- Quantum Computing
- Catalysis
- Polymer Chemistry
- Materials Chemistry
- Data Science

Even though any mix-and-match courses combination is possible, students are strongly advised to consult respective faculty-advisor and/or program coordinator before enrolling courses. They will guide you through registration to realize your further study plans and career goals.

#### **Course Time-Distribution**

Credit weightage of the courses are described in accordance with CBCS regulations of the University and UGC's recommendations. This document deliberately does not specify unitwise time distribution with an intention to allow flexibility to the course tutors. Course tutors are expected to allocate and distribute the time among various units of the courses as per the requirement of the course content and students' comprehension.

## 3. Duration of the Programme

The duration of the UG programme is 4 years or 8 semesters. Students who desire to undergo a 3-year UG Programme will be allowed to exit after completion of the 3<sup>rd</sup> year. If a student wants to leave after the completion of the first or second year, the student will be given a UG Certificate or UG Diploma, respectively, provided they secure the prescribed number of credits (as given in table below). Students who exit with a UG certificate or UG diploma are permitted to re-enter within three years and complete the degree programme. Students may be permitted to take a break from the study, they are allowed to re-enter the degree programme within 3 years and complete the programme within the stipulated maximum period of seven years.

## 4. Eligibility for the UG Programmes

Senior Secondary School Leaving Certificate or Higher Secondary (12<sup>th</sup> Grade) Certificate obtained after successful completion of Grade 12 or equivalent stage of education corresponding to Level-4 (Levels in NHEQF).

## 5. Awarding of UG Certificate, UG Diploma, and Degrees

**UG Certificate**: Students who opt to exit after completion of the first year and have earned a minimum of 42 credits will be awarded a UG certificate if, in addition, they complete work based vocational course/internship of 4 credits during the summer vacation of the first year.

**UG Diploma**: Students who opt to exit after completion of the second year and have earned a minimum of 84 credits will be awarded the UG diploma if, in addition, they complete wok based vocational course/internship of 4 credits during the summer vacation of the second year.

**3-year UG Degree:** Students who wish to discontinue after the 3- year UG programme will be awarded a UG Degree in the Major discipline after successful completion of three years, earning a minimum of 124 credits and satisfying the minimum credit requirements as mentioned in the table below.

**4-year UG Degree (Honours):** A four-year UG Honours degree in the major discipline will be awarded to those who complete a four-year degree programme, earning a minimum of 164 credits and have satisfied the credit requirements as mentioned in table below.

**4-year UG Degree (Honours with Research):** Students who secure a minimum of 7.5 CGPA in the first six semesters and wish to undertake research at the undergraduate level can choose a research stream in the fourth year. They should do a research project or dissertation under the guidance of a faculty member of the University. The research project/dissertation will be in the major discipline. The students who secure a minimum of 164 credits, including 12 credits from a research project/dissertation, will be awarded UG Degree (Honours with Research).

## 6. Structure of the Undergraduate Programme

Every Integrated Programme offered by the University shall confirm to the structure specified hereunder. A programme must mandate the students to complete 124 credits to complete a basic Bachelor's Degree within the first 3 years. With an additional 40 credits of course work one can pursue 4<sup>th</sup> Year Honours or Honours with Research Degree. The UG Programme will consist of the following categories of courses and the minimum credit requirements for 3-year UG and 4-year UG (Honours) or UG (Honours with Research) programmes are given below.

## 7. Program Credit Requirements

Major Discipline – Chemistry	60 Credits (15 Courses of 4 credits)	
Minor Disciplinary*/Interdisciplinary	24 Credits (6 Courses of 4 Credits)	
Courses (Vocational Programme		
included)		
Multi-Disciplinary Courses	9 Credits (3 courses of 3 credits)	
Ability Enhancement Courses	12 Credits (4 courses of 3 credits)	
Skill Enhancement Course	9 Credits (3 courses of 3 credits)	
Value-added courses	8 Credits (4 courses of 2 credits)	
Summer Internship	4 Credits (included in Major courses of 60 credits)	
Community Engagement and Service	2 Credits (1 course)	
Research Dissertation Project	Nil	

#### 3-Years B.Sc. Chemistry Program [Credit Requirement: 124]

#### 4-Years B.Sc. (Hons.) Chemistry Program [Credit Requirement: 164]

Major Discipline – Chemistry	92 Credits (20 Courses of 4 credits)
Minor Disciplinary*/Interdisciplinary	32 Credits (8 Courses of 4 credits)
Courses (Vocational Programme	
included)	
Multi-Disciplinary Courses	9 Credits (3 courses of 3 credits)
Ability Enhancement Courses	12 Credits (4 courses of 3 credits)
Skill Enhancement Course	9 Credits (3courses of 3 credits)
Value-added courses	8 Credits (4 courses of 2 credits)
Summer Internship	4 Credits (included in Major courses of 80 credits)
Community Engagement and Service	2 Credits (1 course)
Research Dissertation Project	Nil

#### **4-Years B.Sc. (Hons. with Research) Chemistry Program [Credit Requirement: 164]**

(Note: Students who secure a minimum of 7.5 CGPA in the first six semesters are eligible for this program)

Major Discipline – Chemistry	80 Credits (20 Courses of 4 credits)
Minor Disciplinary*/Interdisciplinary	32 Credits (8 Courses of 4 credits)
Courses (Vocational Programme	
included)	
Multi-Disciplinary Courses	9 Credits (3 courses of 3 credits)
Ability Enhancement Courses	12 Credits (4 courses of 3 credits)
Skill Enhancement Course	9 Credits (3courses of 3 credits)
Value-added courses	8 Credits (4 courses of 2 credits)
Summer Internship	4 Credits (included in Major courses of 80 credits)
Community Engagement and Service	2 Credits (1 course)
Research Dissertation Project	12 Credits

#### 4-Years B.Sc. (Hons. with Research) Chemistry (Specialization – Chemical Biology) [Credit Requirement: 164]

(This can be taken as a template for other specialization)		
	Cleansisters	90 Credits (20 Courses of 4 and its)

Major Discipline – Chemistry	80 Credits (20 Courses of 4 credits)	
Minor Disciplinary*/Interdisciplinary	32 Credits (8 Courses of 4 credits) in which	
Courses (Vocational Programme	minimum of 12 credits from Chemical Biology	
included)	Specialization)	
Multi-Disciplinary Courses	9 Credits (3 courses of 3 credits)	
Ability Enhancement Courses	12 Credits (4 courses of 3 credits)	
Skill Enhancement Course	9 Credits (3courses of 3 credits)	
Value-added courses	8 Credits (4 courses of 2 credits)	
Summer Internship	4 Credits (included in Major courses of 80 credits)	
Community Engagement and Service	2 Credits (1 course)	
**Research Dissertation Project	12 Credits	

- \* 40% of the credits of minor courses may be earned through online mode (Swayam or such other similar platforms) approved by the department and the University as per the existing UGC regulations. Such decisions may be taken by the department/centres after considering the course requirements and learning outcomes planned and duly approved by the Programme Committee. This does not apply to the major courses/internship/skill enhancement courses/community service/engagement or any other hands-on/vocational programs. Such courses need to be completed offline/physical mode.
- \*\* a. Students who secure a minimum of 7.5 CGPA in the first six semesters are eligible to undertake Research Dissertation Project
  - b. 4 Years B.Sc. (Hons.) Chemistry (Specialization Chemical Biology) students not undertaking research will do 3 major courses for 12 credits in lieu of a Research Project/Dissertation.

## 8. Exit Options

Certification	Normal Residency	Credit	Additional
	Requirements	Requirements	Requirements
Certificate in Chemistry	After 2-Semesters of Study	42 Credits	Work Based Internship – 4 Credits/ Skill Development – 4 Credits
Diploma in Chemistry	After 4-Semesters of Study	84 Credits	Work Based Internship – 4 Credits/ Skill Development – 4 Credits
B.Sc. Chemistry	After 6-Semesters of Study	124 Credits	
B.Sc. (Hons.) Chemistry	After 8-Semesters of Study	164 Credits	
B.Sc. (Hons. with Research) Chemistry*	After 8-Semesters of Study	164 Credits Including Undergraduate Research Project and Thesis Submission	

\* Only students who secure a CGPA of 7.5 and above in the previous 124 credits (*B.Sc. Chemistry*) are allowed to enroll.

## 9. Semester-wise Course/Credit Distribution

Semester-wise credit distribution for 4-years B.Sc. (Hons.)/ B.Sc. (Hons., with Research) Chemistry program is shown below. Since various schools/departments/centers are involved in offering courses, the department may reorganize semester credits as per the availability of human resources and infra-structure facilities.

<b>Course Code</b>	Course Title	Туре	Credits
<b>CHEM 1101</b>	General Chemistry – I: Molecular Geometry & Shapes	Major Discipline-1	4
CHEM 1102	Essentials of Chemistry – I:	Minor Discipline-1	4
CHEM 1103	Introduction to Chemistry – I	MD-1 (Natural Science – 1)	3
<b>CHEM 1100</b>	Chemistry Laboratory – I	SEC-1	3
	English – I	AEC-1	3
	Environmental Science	VAC-1	2
	Understanding India	VAC-2	2

#### Semester I (21 – Credits)

#### Semester II (21 Credits)

<b>Course Code</b>	Course Title	Туре	Credits
<b>CHEM 1201</b>	General Chemistry – II	Major Discipline-2	4
<b>CHEM 1202</b>	Essentials of Chemistry – II	Minor Discipline-2	4
CHEM 1203	Introduction to Chemistry – II	MD-2 (Natural Science – 2)	3
<b>CHEM 1200</b>	Chemistry Laboratory – II	SEC-2	3
	Sanskrit/Hindi/Tamil/French Languages (to be chosen by the student)	MIL-1	3
	Health & Well-being Yoga	VAC-3	2
	Digital Technological Solution	VAC-4	2

### Semester III (21 Credits)

<b>Course Code</b>	Course Title	Туре	Credits
<b>CHEM 2101</b>	General Chemistry – III	Major Discipline-3	4
CHEM 2102	General Chemistry – IV	Major Discipline-4	4
CHEM 2103	Introduction to Chemistry – III	MD-3 (Natural Science – 3)	3
<b>CHEM 2104</b>	Practice of Chemistry – I	Minor Discipline-3	4
<b>CHEM 2100</b>	Chemistry Laboratory – III	SEC-3	3
	English – 2	AEC-2	3

#### Semester IV (21 Credits)

Course Code	Course Title	Туре	Credits
<b>CHEM 2201</b>	Inorganic Chemistry – I:	Major Discipline-5	4
	Miscellaneous topics		
CHEM 2202	Organic Chemistry – I: Functional	Major Discipline-6	4
	Group Transformations		
CHEM 2203	Physical Chemistry – I: Atomic	Major Discipline-7	4
	Structure and Bonding		
<b>CHEM 2204</b>	Practice of Chemistry – II	Minor Discipline-4	4
	Sanskrit/Hindi/Tamil/French	MIL-2	3
	Languages (to be chosen by the		
	student)		
	Community Engagement/Service	VAC-5	2

### Semester V (20 Credits)

<b>Course Code</b>	Course Title	Туре	Credits
<b>CHEM 3101</b>	Inorganic Chemistry – II: Chemistry	Major Discipline-8	4
	of transition metal complexes		
CHEM 3102	Organic Chemistry – II: Synthetic	Major Discipline-9	4
	methods, Polymers and Spectroscopic		
	Techniques		
CHEM 3103	Physical Chemistry – II: Reaction	Major Discipline-10	4
	Energetics		
<b>CHEM 3104</b>	Practice of Chemistry – III	Minor Discipline-5	4
<b>CHEM 3100</b>	Internship	Major Discipline-11	4

#### Semester VI (20 Credits)

<b>Course Code</b>	Course Title	Туре	Credits
CHEM 3201	Inorganic Chemistry – III:	Major Discipline-12	4
	Organometallics and Bio-inorganic		
	Chemistry		
CHEM 3202	Organic Chemistry – III: Heterocycles,	Major Discipline-13	4
	Biomolecules and Drugs		
CHEM 3203	Physical Chemistry – III: Reaction	Major Discipline-14	4
	Kinetics		
CHEM 3204	Topics in Analytical Chemistry	Major Discipline-15	4
CHEM 3205	Selected Topics in Inorganic Chemistry	Minor Discipline-6	4

#### Semester VII (20 Credits)

Course Code	Course Title	Туре	Credits
<b>CHEM 4101</b>	Inorganic Chemistry – IV: Advanced	Major Discipline-16	4
	Main group Chemistry and Inorganic		
	Spectroscopy		
CHEM 4102	Organic Chemistry – IV: Spectroscopic	Major Discipline-17	4
	Identification of Organic Compounds		
<b>CHEM 4103</b>	Physical Chemistry – IV: Principles of	Major Discipline-18	4
	Spectroscopy		
CHEM 4104	Selected Topics in Organic Chemistry	Minor Discipline-7	4
CHEM 4105	Selected Topics in Physical Chemistry	Minor Discipline-8	4

#### Semester VIII (20 Credits)

Course Code	Course Title	Туре	Credits
CHEM 4201 to	To be offered by the faculty members	Major Discipline-19	4
<b>CHEM 4218</b>	and will be chosen by the students		
CHEM 4201 to	To be offered by the faculty members	Major Discipline-20	4
<b>CHEM 4218</b>	and will be chosen by the students		
CHEM 4201 to	To be offered by the faculty members	Major Discipline-21	4*
<b>CHEM 4218</b>	and will be chosen by the students		
CHEM 4201 to	To be offered by the faculty members	Major Discipline-22	4*
<b>CHEM 4218</b>	and will be chosen by the students		
CHEM 4201 to	To be offered by the faculty members	Major Discipline-23	4*
<b>CHEM 4218</b>	and will be chosen by the students		
<b>CHEM 4200</b>	Research Project and Dissertation	Major Discipline-24	12**
		(for Honors with	
		research)	

\*For the students who do not undertake the research project.

\*\*For those who go for the research stream need to take only two theory courses.

## **10. Description of Courses**

The following are the types of courses in the UG Programme.

#### Major Discipline (60 to 80 Credits)

Major discipline is the discipline or subject of main focus and the degree will be awarded in that discipline. Students should secure the prescribed number of credits (not less than 50% of the total credits) through core courses in the major discipline. The major discipline would provide the opportunity for a student to pursue in-depth study of a particular subject or discipline. A student may choose to change the major discipline within the broad discipline at the end of the second semester provided all the prerequisites of the respective degree programme are fulfilled.

#### Minor Discipline (24 to 32 credits)

Minor discipline helps a student to gain a broader understanding beyond the major discipline. For example, if a student pursuing an Economics major obtains a minimum of 12 credits from a bunch of courses in Statistics, then the student will be awarded

B.A. degree in Economics with a Minor in Statistics.

- 24 credits of minor courses in the 3-year programme can be Disciplinary or Interdisciplinary courses or a mix of both. 50% of the total credits from minors must be secured in the relevant subject/discipline and another 50% of the total credits can be from any discipline of students' choice.
- 12 credits (50%) of the Minor (Disciplinary / Interdisciplinary) in the 3-year programme should be related to vocational education/training courses.

Type of Minor	Credits
Disciplinary/Interdisciplinary	12
Disciplinary/Interdisciplinary vocational	12

#### Multi-disciplinary Courses (MD): 9 credits

All UG students are required to undergo 3 introductory-level courses relating to any of the broad disciplines given below. These courses are designed and developed by every department for the benefit of other discipline students and are pooled by SAMS under 5 baskets for students to choose any 3 courses from 3 broader areas (one each from any three broad areas from below) from the basket. Students are not allowed to choose or repeat courses already undergone at the higher secondary level (12th class) under this category.

- a. *Natural and Physical Sciences:* Students can choose basic courses from disciplines such as Natural Science, for example, Biology, Botany, Zoology, Biotechnology, Biochemistry, Chemistry, Physics, Biophysics, Astronomy and Astrophysics, Earth and Environmental Sciences, and other related subjects.
- b. *Mathematics, Statistics, and Computer Applications:* Courses under this category will facilitate the students to use and apply tools and techniques in their major and minor disciplines. The course may include training in programming software like Python among others and applications software like STATA, SPSS, Tally and similar others. Basic

courses under this category will be helpful for science and social science in data analysis and the application of quantitative tools.

- c. Library, Information, and Media Sciences: Courses from this category will help the students to understand the recent developments in information and media science (journalism, mass media, and communication)
- d. *Commerce and Management:* Courses include business management, accountancy, finance, financial institutions, fintech and other related subjects.
- e. *Humanities and Social Sciences:* The courses relating to Social Sciences, for example, Anthropology, Communication and Media, Economics, History, Linguistics, Political Science, Psychology, Social Work, Sociology and other related subjects will enable students to understand the individuals and their social behaviour, society, and nation. Students be introduced to survey methodology and available large-scale databases for India. The list of Courses that can include interdisciplinary subjects such as Cognitive Science, Environmental Science, Gender Studies, Global Environment & Health, International Relations, Political Economy and Development, Sustainable Development, Women's and Gender Studies and similar subjects. will be useful to understand society.

Note: As explained elsewhere in this regulation, all departments/centres/schools are mandated to participate in the conduct of these courses and offer at least one introductory course on the concerned subjects, in the above groups and the students can choose these subjects from the basket of courses.

#### Ability Enhancement Courses (AEC): 12 credits

Modern Indian Language (MIL) & English language focused on language and communication skills.

Students are required to achieve competency in a Modern Indian Language (MIL) and in the English language with special emphasis on language and communication skills. The courses aim at enabling the students to acquire and demonstrate the core linguistic skills, including critical reading and expository and academic writing skills, that help students articulate their arguments and present their thinking clearly and coherently and acquaint with the cultural and intellectual heritage of languages.

#### Skill Enhancement Courses (SEC): 9 credits

These courses are aimed at imparting practical skills, hands-on training, soft skills, and other skills to enhance the employability of students. The institution may design courses as per the students' needs and available institutional resources. Skill based courses could be related to disciplinary/interdisciplinary minors and vocational education programmes chosen/offered.

#### Value-Added Courses (VAC) Common to All UG Students: 8 credits

a. *Understanding India:* This course aims at enabling the students to acquire and demonstrate the knowledge and understanding of contemporary India with its historical perspective, the basic framework of the goals and policies of national development, and the constitutional obligations with special emphasis on constitutional values and fundamental rights and duties. The course would also focus on developing an

understanding among student- teachers of the Indian knowledge systems, the Indian education system, and the roles and obligations of teachers to the nation in general and to the school/community/society. The course will attempt to deepen knowledge about and understanding of India's freedom struggle and of the values and ideals that it represented to develop an appreciation of the contributions made by people of all sections and regions of the country, and help learners understand and cherish the values enshrined in the Indian Constitution and to prepare them for their roles and responsibilities as effective citizens of a democratic society.

- b. *Environmental Science/Education:* This course seeks to equip students with the ability to apply the acquired knowledge, skills, attitudes, and values required to take appropriate actions for mitigating the effects of environmental degradation, climate change, and pollution, effective waste management, conservation of biological diversity, management of biological resources, forest and wildlife conservation, and sustainable development and living. The course will also deepen the knowledge and understanding of India's environment in its totality, its interactive processes, and its effects on the future quality of people's lives.
- c. *Digital and Technological Solutions*: Courses in cutting- edge areas that are fast gaining prominences, such as Artificial Intelligence (AI), 3-D machining, big data analysis, machine learning, drone technologies, and Deep learning with important applications to health, environment, and sustainable living that will be woven into undergraduate education for enhancing the employability of the youth.
- d. *Health & Wellness, Yoga Education, Sports, and Fitness:* Course components relating to health and wellness seek to promote an optimal state of physical, emotional, intellectual, social, spiritual, and environmental well-being of a person. Sports and fitness activities will be organized outside the regular institutional working hours. Yoga education would focus on preparing the students physically and mentally for the integration of their physical, mental, and spiritual faculties, and equipping them with basic knowledge about one's personality, maintaining self- discipline and self-control, to learn to handle oneself well in all life situations.

#### **Vocational Training/Education: 12 Credits**

These courses are meant to provide the students with adequate knowledge and skills for employment and entrepreneurship. Departments are expected to incorporate the requirements of related industries while designing these courses to groom the students to take up gainful employment or becoming entrepreneurs. Vocational education courses designed by each department should relate the skills provided with the content of general education in order to ready the students for work at each exit point of the programme. A minimum of 12 credits will be allotted to the minor stream relating to vocational education and training.

#### **Summer Internship: 4 Credits**

All students will undergo internships / Apprenticeships in a firm, industry, or organization or Training in labs with faculty and researchers in their own or other HEIs/research institutions during the summer term. Students will be provided with opportunities for internships to

actively engage with the practical side of their learning and, as a by-product, further improve their employability. Summer internship shall be conducted for a minimum of 8 weeks.

#### **Community Engagement and Service: 2 Credits**

The curricular component of 'community engagement and service' seeks to expose students to the socio-economic issues in society so that the theoretical learnings can be supplemented by actual life experiences to generate solutions to real-life problems. This can be part of summer term activity or part of a major or minor course depending upon the major discipline. Community Engagement shall be conducted for a minimum of 2 weeks.

#### **Research Project / Dissertation: 12 Credits**

Students choosing a 4-Year Bachelor's degree (Honors with Research) are required to take up research projects under the guidance of a faculty member. The students are expected to complete the Research Project in the eighth semester.

#### Audit courses: 0 credits

Audit courses offered do not carry any credits. Evaluation will be based on continuous assessment. Students may be given a pass or fail (P/F) based on the assessment that may consist of class tests, homework assignments, and/or any other innovative assessment methodology suitable to the expected learning outcome, as determined by the faculty in charge of the course of study.

## 11. Credit-hours for Different Types of Courses

A three-credit lecture course in a semester means three one-hour lectures per week with each one-hour lecture counted as one credit. One credit for tutorial work means one hour of engagement per week.

A one-credit course in practicum or lab work, community engagement and services, and fieldwork in a semester mean two-hour engagement per week. In a semester of 15 weeks duration, a one-credit practicum in a course is equivalent to 30 hours of engagement. A one-credit of Seminar or Internship or Studio activities or Field practice/projects or Community engagement and service means two-hour engagements per week. Accordingly, in a semester of 15 weeks duration, one credit in these courses is equivalent to 30 hours of engagement.

- *Lecture courses:* Courses involving lectures relating to a field or discipline by an expert or qualified personnel in a field of learning, work/vocation or professional practice
- *Tutorial:* Courses involving problem solving and discussions relating to a field or discipline.
- *Seminar:* A course requiring students to participate in structured discussion/conversation or debate focused on assigned tasks/readings, current or historical events, or shared experiences guided or led by an expert or qualified personnel in a field of learning, work/vocation or professional practice.
- *Practicum:* A course requiring students to participate inan approved project or practical activity that applies previously learned/studied principles/theory related to the chosen field of learning, work/vocation or professional practice.

- *Internship:* A course requiring students to participate in professional employment• related activity or work experience, or cooperative education activity with an entity external to the education institution, normally under the supervision of an employee of the given external entity.
- *Laboratory work/activity:* A course requiring students to discover/practice application of a scientific or technical principles/theories. The course may require scientific, or research focused experiential work where students observe, test, conduct experiment(s) or practice application of principles/theories relating to field of learning, work/vocation or professional practice.
- *Studio activities:* Studio activities involve engagement of students in creative or artistic activities. Studio-based activities involve visual- or aesthetic-focused experiential work.
- *Workshop-based activities:* Courses involving workshop- based activities requiring engagement of students in hands- on activities related to work/vocation or professional practice.
- *Field practice/projects:* Courses requiring students to participate in field-based learning/project generally under the supervision of an employee of the given external entity.

## 12. Programmes of Study, Eligibility and Graduating Requirements - Admissions by Lateral Entry

In all Academic programmes where admission was carried out adopting approved procedures in preceding years, subject to availability, lateral entry admission shall be permitted, subject to:

- a. that the University shall notify the admission process and number of vacancies open for lateral entry.
- b. that the Lateral entrants shall be admitted only after such transparent screening process and such procedure that the University may prescribe from time to time. University may prescribe different methods of screening for different programmes depending on the circumstances prevailing in each case.
- c. Lateral entry shall be permissible only in the beginning of years 2,3,4 of the Under Graduate/honours programme; provided that students seeking lateral entry shall have obtained the minimum pass marks/ grades fixed by the University in their previous academic years.

## 13. Degrees, Diplomas and Certificates of the University and Minimum Credit Requirements

The University shall award Degrees, Diplomas and Certificates as follows:

a. A Bachelor's with Honours/Honours with Research Degree in the discipline of the candidate (appropriately styled) who has earned at least 164 credits in 4 years; and a basic Bachelor's Degree in the given discipline of the candidate (appropriately styled) for those

who have earned at least 124 credits including NEP specified courses, during first 3 years of academic programme.

- b. A Diploma for those students who have earned at least 84 credits including the NEP specified courses and the mandatory 4 credits of skill enhancement/internship programmes in the summer semester.
- c. A Certificate for those students who have earned at least 42 credits including the NEP specific courses and the mandatory 4 credits of skill enhancement/internship programmes.

## 14. Academic Bank of Credits (ABC)

The scheme of academic bank of credits will facilitate the transfer and consolidation of credits by using an 'academic bank account' opened by students across the country by taking up courses in any of the eligible HEIs. The validity of the credits earned and kept in the academic credit account will be to a maximum period of seven years or as specified by the ABC time to time.

## 15. Minimum Credits for Enrolment, Online Courses, Student Strength and Mentorship

- a. To be considered a full-time student, a student must be enrolled at least for 12 credits in each and every Semester. No student, unless specifically permitted by the Programme committee, be permitted to enroll in more than 30 credits in any semester (excluding the credits for writing arrear exams).
- b. 40% of the credits of minor courses may be earned through online mode (Swayam or such other similar platforms) approved by the department and the University as per the existing UGC regulations. Such decisions may be taken by the department/centres after considering the course requirements and learning outcomes planned and duly approved by the Programme Committee. This does not apply to the major courses/internship/skill enhancement courses/community service/engagement or any other hands-on/vocational programmes. Such courses need to be completed offline/physical mode.
- c. Course code for online courses and the number of credits assigned to each course will be approved by the programme committee of respective department/Centre, and these will be uploaded in the PU-SAMS portal.
- d. A student will be permitted to register for only one minor course during one semester.
- e. Students will be permitted to drop online courses within the time limits prescribed in the Academic Calendar.
- f. Every student upon admission to the University shall be associated with a member of the faculty of the programme to which she/he is admitted to, who shall advise and help the student as a mentor in choosing courses that is most appropriate for the goals of the student.
- g. No minor course shall be offered unless a minimum of 10 students are registered.

## 16. Exit Options Description

- a. Students enrolled in any Programme shall have an option to exit at the end of 1<sup>st</sup>, 2<sup>nd</sup> and 3<sup>rd</sup> years of a programme, subject to fulfilment of conditions.
- b. A student desiring an exit shall give a notice of such intention in writing in the prescribed format at least 8 weeks before the scheduled end of the Academic year.
- c. The Department running the programme shall on receipt of the notice shall recommend for a Certificate/ Diploma/ Degree as the case may be from the University based on the requirements for such degrees. In case of arrear papers, the certificate shall be provided after passing the arrear paper.
- d. As soon as the student completes the requirements of the certificate/diploma/degree, as the case may be, the Department shall communicate to such officer as may be notified by the Administration.

#### **17.** Learning Assessment

Continuous Assessment and End Semester Examination marks and evaluation of skill based/vocational courses/ Internships and other hands on/field-based courses

- All theory courses in a UG programme shall carry a continuous assessment component of 40 marks and end semester assessment component of 60 marks.
- In case of skill-based courses, vocational education courses, internships, practical, lab/field/project works, community service and related skill-based activities, the evaluation pattern may be decided by the respective Programme Committees/BOS and be approved in Academic Council. The evaluation methods need to be drawn based on the learning outcomes planned for such courses following the NEP guidelines of Pondicherry University.

#### **Continuous Assessment Component (Sessional)**

- Evaluation will be based on continuous assessment carried out through activities spread over a complete semester based on the learning outcomes listed. Sessional work consists of class tests, at least one mid-semester examination, homework assignments, and any other innovative assessment methodology as determined by the faculty in charge of the course of study. Progress towards achievement of learning outcomes shall be assessed using the following: time-constrained examinations; closed-book and open-book tests; problem-based assignments; practical assignments; laboratory reports; observation of practical skills; individual project reports (case-study reports); team project reports; oral presentations, including seminar presentation; viva voce interviews; computerized adaptive assessments, examination on demand, modular certifications and other suitable assessments methods.
- Total Marks from continuous assessments may be up to 40% of the total. Departments/Centres/Schools need to design suitable continuous assessment models splitting the 40 marks into 2 to 4 different components including at least one mid semester test, duly approved by the PC/BOS. This splitting may match the requirements/nature of courses taught.

#### **End- Semester Examination and Evaluation**

- End semester examinations shall be conducted for all courses offered in the department/centres after ensuring that the required number of classes and related activities are completed. The duration of the end semester examination may be 3 hours.
- A schedule of End semester examinations will be announced by the department/centre about 15 days ahead of the conduct of examinations.
- The responsibility of question paper setting, invigilation and valuation of answer papers lie with the course teachers. However, all assessments shall be conducted under the uniform practices of the department approved in the programme committee.
- However, the departments/faculty members are free to decide the components of continuous assessment and the method of assessment based on the nature of the course and are expected to communicate these to students and respective HODs at the beginning of the semester.
- Mid semester /end semester examinations schedule notified by the University in the academic calendar shall be uniformly followed.

#### **Minimum Marks for Pass**

A student shall be declared to have passed the course only if she/he gets,

- A minimum of 40% marks in End Semester Exam and
- A minimum of 40% marks in aggregate when continuous assessment and end semester examination marks are put together.

#### **Supplementary Examination**

- A student who gets F grade in a course shall be permitted to register for the supplementary examination in the following semester or in the subsequent semesters.
- A student who gets F grade in a course shall be given an option either to retain the previously awarded continuous assessment mark or to improve it, and the higher mark out of these two options will be considered for the supplementary examination.
- A student who gets Ab grade in a course/practicum/vocational course/ internship/practicum or any other hands-on skill related course is mandated to repeat the course and undergo all the stages of assessment in subsequent semesters.

## 18. Attendance Requirement

No student who has less than 70% attendance in any course shall be permitted to participate in end semester examination and she/he shall be given 'Ab' grade, -failure due to lack of attendance. she/he shall be required to repeat that course as and when it is offered.

## **19. Letter Grades and Grade Points**

Performance of students in each paper will be expressed as marks as well as Letter Grades.

Letter Grade	Grade Point
O (Outstanding)	10
A+ (Excellent)	9
A (Very good)	8
B+ (Good)	7
B (Above average)	6
C (Average)	5
P (Pass)	4
F (Fail)	0
Ab (Absent)	0

In case of fractions the marks shall be rounded off to nearest integer. The class interval K will be calculated by the formula given below:

# K = (X-50)/6 where X is the highest mark secured.

According to K value, one of the following grading scheme will be followed.

(i) If  $K \ge 5$ , then the grades shall be awarded as given in Table II.

Table II			
Range of Marks in %	Letter Grade	Letter Grade	
	<b>Points for</b>	Points for	
X to (X-K)+1	0	10	
(X-K) to (X-2K)+1	A+	9	
(X-2K) to (X-3K)+1	А	8	
(X-3K) to (X-4K)+1	B+	7	
(X-4K) to (X-5K)+1	В	6	
(X-5K) to 50	С	5	
40-49	Р	4	
Below 40	F	0	
Absent (Lack of Attendance)	Ab	0	

Table III					
Range of Marks in %	Letter Grade Points for	Letter Grade Points for			
80-100	0	10			
71-79	A+	9			
66-70	А	8			
61-65	B+	7			
56-60	В	6			
50-55	С	5			
40-49	Р	4			
Below 40	F	0			
Absent (lack of attendance)	Ab	0			

(ii) If K<5, then the grades shall be awarded as given in Table III.

The Semester Grade Point Average (SGPA) is computed from the grades as a measure of the student's performance in a given semester. The SGPA is based on the grades of the current term, while the Cumulative GPA (CGPA) is based on the grades in all courses taken after joining the programme of study.

## 20. Computation of SGPA and CGPA

The following procedure shall be followed to compute the Semester Grade Point Average (SGPA) and Cumulative Grade Point Average (CGPA):

The SGPA is the ratio of the sum of the product of the number of credits with the grade points scored by a student in all the courses taken by a student and the sum of the number of credits of all the courses undergone by a student, i.e. **SGPA** (Si) =  $\Sigma$ (Ci x Gi) /  $\Sigma$ Ci

Where Ci is the number of credits of the  $i^{th}$  course and Gi is the grade point scored by the student in the  $i^{th}$  course.

Semester	Course	Credit	Letter Grade	Grade point	<b>Credit Point</b> (Credit x Grade)
				-	
Ι	Course 1	3	А	8	3 X 8 = 24
Ι	Course 2	4	B+	7	4 X 7 = 28
Ι	Course 3	3	В	6	3 X 6 = 18
Ι	Course 4	3	0	10	3 X 10 = 30
Ι	Course 5	3	С	5	3 X 5 = 15
Ι	Course 6	4	В	6	4 X 6 = 24
		20			139
				SGPA	139/20=6.95

Example for Computation of SGPA where candidate has not failed in any course.

Semester	Course	Credit	Letter Grade	Grade point	<b>Credit Point</b> (Credit x Grade)
Ι	Course 1	3	А	8	3 X 8 = 24
Ι	Course 2	4	B+	7	4 X 7 = 28
Ι	Course 3	3	В	6	3 X 6 = 18
Ι	Course 4	3	0	10	3 X 10 = 30
Ι	Course 5	3	С	5	3 X 5 = 15
Ι	Course 6	4	F	0	$4 \ge 0 = 00$
		20			115
			•	SGPA	115/20=5.75

#### (i) Example for Computation of SGPA where candidate has failed in one course.

#### (ii) Example for Computation of SGPA where candidate has failed in two courses.

			Letter	Grade	Credit Point
Semester	Course	Credit	Grade	point	(Credit x Grade)
T	0 1	2		0	<b>A X A</b>
I	Course I	3	A	8	3 X 8 = 24
Ι	Course 2	4	B+	7	4 X 7 = 28
Ι	Course 3	3	F	0	$3 \ge 0 = 00$
Ι	Course 4	3	В	6	3 X 6 = 18
Ι	Course 5	3	С	5	3 X 5 = 15
Ι	Course 6	4	F	0	$4 \ge 0 = 00$
		20			85
				SGPA	85/20=4.25

The CGPA shall also be calculated in similar way as shown in examples (i), (ii) and (iii) of SGPA for all subjects taken by the students in all the semesters. However, if any student fails more than once in the same subject, then while calculating CGPA, the credit and grade point related to the subject in which the student fails in multiple attempts will be restricted to one time only. The SGPA and CGPA shall be rounded off to 2 decimal points and reported in the transcripts.

In case of audit courses offered, the students may be given (P) or (F) grade without any credits. This may be indicated in the mark sheet. Audit courses will not be considered towards the calculation of CGPA.

## 21. Grade Card

The University shall issue a Grade card for the students, containing the marks and grades obtained by the student in the previous Semester Grade Point Average (SGPA) and Cumulative Grade Point Average (CGPA).

The grade card shall list:

a. The title, semester and course code of the courses taken by the student.

- b. The credits associated with the course.
- c. The marks and grade secured by the student.
- d. The total credits earned by the student in that semester
- e. The SGPA of the student.
- f. The total credits earned by the students till that semester.
- g. The CPGA of the student.

On successful completion of the programme, students with a CGPA of 9.00 and above who passed all the courses in the first attempt shall be awarded the degree in First Class with Distinction. University Rank in a programme will be awarded to the student who secures the highest CGPA in a batch and passed all the courses in first attempt. Students with CGPA between 6.00 and 8.99 shall be placed in First Class, students with CGPA between 5.00 and 5.99 shall be placed in Second Class, and students with CGPA between 4.00 and 4.99 shall be placed in Pass Class.

**22. Syllabus for Major Courses** 

#### Major 1

#### CHEM 1101 General Chemistry I: Molecular Geometry & Shapes

**Learning** Molecular stereochemistry is a fundamental aspect of all areas of chemistry. To understand the nature of bonding between elements. To realize the three-dimensional structure of molecules.

**Learning** This course enables the students (a) to identify and assign shapes and molecular symmetry elements (b) to visualize, identify, evaluate, 3D molecular structures and energetics of isomers (c) to understand the structural features of solids

#### **Course Content:**

#### **Unit I – Classical Bonding:**

Types of bonds, representation of electrons as dots, Lewis model of ionic, covalent structures, Electronegativity and bond polarity, Lewis structure of molecular compounds, formal charge, exception to octet rule, bond energies and bond lengths, bonding in metals – VSEPR theory, predicting molecular geometry, shapes and polarity – Valence Bond theory – Molecular orbital theory, electron delocalization.

#### Unit II – Bonding in Organic Molecules:

Bonding and shapes of organic molecules – hybridization, oxidation number, resonance – delocalization of electrons; inductive effect, introduction to functional groups, intermolecular forces, Brønsted–Lowry acids and bases – pKa & pKb, effect of structure on acidity, HSAB principle, Nomenclature of organic compounds.

#### Unit III – Basics of Stereochemistry:

Types of isomers – constitutional isomers and stereoisomers; representation of stereoisomers – Fischer projection, saw-horse projection, Newman projection formulae, configurational isomers, geometrical isomers, conformational isomers – ethane, butane, cyclohexane.

#### **Unit IV – Stereochemistry of Inorganic Compounds:**

Geometrical and optical nature of 4-, 5-, 6- coordinated p-block and transition elements compounds having mono-, di-, tri-dentate ligands; stereochemistry of 7- and above coordination compounds.

#### **Unit V – Point Groups of Molecules:**

Symmetry elements and operations, assignment of point groups for chemical molecules with examples.

#### **Textbook:**

- 1. Organic Chemistry, P. Y. Bruice, Pearson Education, 7th Edn, 2013
- 2. Inorganic Stereochemistry, D. L. Kepert, Springer Verlag, 1982.
- 3. Inorganic Structural Chemistry, U. Muller, 2<sup>nd</sup> Edn., Wiley, 2006.
- 4. Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg (Part A and B) Kluwer Academic / Plenum Publishers, 2000.
- 5. Organic Stereochemistry: Stereochemistry of Organic Compounds, E. L. Eliel, and S. H. Wilen, John Wiley and Sons (Asia) Pvt. Ltd., Singapore, 2003
- 6. F. Albert Cotton, Chemical Applications of Group Theory, 3<sup>rd</sup> Edition, Wiley, 1990.

#### CHEM 1201 General Chemistry II

- **Learning** This course explores the electronic structure of elements starting from hydrogen, alkali and alkaline earth metals, and the basic treatment of boron group elements. It covers the structure and bonding, and functionalization of alkanes. Basic knowledge in quantum mechanics and the solving wave equations are introduced in this course.
- **Learning** The student may be expected to understand the structure and bonding nature of chemical elements and learn different chemical reactions, and also learn to solve the wave equation with quantum mechanical treatment.

#### **Course Content:**

#### Unit I – Hydrogen and Hydrides, Alkali and Alkaline Earth Metals:

Hydrogen and Hydrides: Electronic structure, abundance, preparation and properties, isotopes, orthoand para hydrogen; Hydrides: ionic, covalent, metallic and intermediate hydrides; Hydrogen bonding. Alkali metals: Introduction, halides, oxides and hydroxides, salts of oxo-acids, aqueous solution chemistry, complexes and organometallic compounds. Alkaline Earth metals: Introduction, halides, oxides and hydroxides, salts of oxo-acids, aqueous solution chemistry, complexes and organometallic compounds.

#### Unit II – Boron Group (Basic treatment):

Boron group: Boron compounds, metal borides, halides and complex halides of B, Al, Ga, In and Tl, oxides, oxo-acids, oxo-anions and hydroxides; nitrogen derivatives; Al, Ga, In and Tl salts of oxo-acids and aqueous solution chemistry, organometallic compounds.

#### Unit III – Basics of Organic Reaction Mechanism:

Chemical reactivity and mechanism – energetics – enthalpy, entropy, bond energy, Gibbs free energy, activation energy, kinetic and thermodynamic control, Hammond postulate, principle of microscopic reversibility, types of chemical reaction – bond cleavage, nucleophiles, electrophiles, free radicals, arrow pushing in organic chemistry.

#### Unit IV – Functionalization of Alkanes, Alkenes, Dienes and Alkynes:

Alkanes – source of alkanes, functionalizing alkanes - free radical halogenation and oxidations. Laboratory preparation of alkenes, dienes and alkynes. Functionalizing alkenes, dienes and alkynes - Addition reactions, substitution reactions and cycloaddition reactions.

#### Unit V - Basics of Quantum Mechanics:

Planck's Law – Derivation of Bohr's atom – Merits and Drawbacks – Wave-particle Duality – Uncertainty principle – Wave Equation – Particle in a box – Tunneling – Harmonic Oscillator – Power Series Solutions – Hermite Polynomials - Rigid Rotor – 3D Extensions – Legendre Polynomials and its variants –Spherical harmonics - Energy Spacing and Degeneracies - Quantum Postulates.

#### **Textbooks:**

- 1. Organic Chemistry, P. Y. Bruice, Pearson Education, 7th Edn, 2013
- 2. A. G. Sharpe, Inorganic Chemistry, 3<sup>rd</sup> Edition, Addison-Wesley, 1999.
- 3. J. D. Lee, A New Concise Inorganic Chemistry, 3<sup>rd</sup> Edition., ELBS, 1987.
- 4. D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, ELBS. 1990
- 5. D. A. McQuarrie & J. D. Simon, Physical Chemistry: A Molecular Approach, University Science Books, CA, 1997.

#### Major 3

#### CHEM 2101 General Chemistry III

**Learning** This course explores the basic treatment of carbon and oxygen group elements and functionalization of simple organic molecules, and give insights to understand the thermodynamic aspects of chemical reaction and the phase diagrams.

**Learning** The students may understand and write mechanisms for various chemical reactions and able to understand the equilibrium reactions in thermodynamic perspective.

#### **Course Content:**

#### Unit I – Carbon Group (Basic treatment):

Introduction, Intercalation compounds of graphite, carbides and silicides, halides and complex halides; oxides and oxo-acids of carbon; oxides and oxo-acids and hydroxides of Si, Ge, Sn and Pb; Silicates; Silicones; Sulphides; Cyanogen, its derivatives and silicon nitride; aqueous solution chemistry and oxo-acid salts of Sn and Pb; Organometallic compounds.

#### Unit II – Oxygen Group (Basic treatment):

Introduction of Chalcogens; Hydrides; Oxides, Oxo-acids, Halides, Oxo-halides and complex halides, and their salts; Sulphides, Selenides, Tellurides; Aqueous solution chemistry; Nonaqueous SO<sub>2</sub>.

#### **Unit III – Chemistry of Selected Functionalization Groups:**

Chemistry of alkyl halides, alcohols, aldehydes, carboxylic acids and derivatives, amines, thiols and nitro compounds.

#### **Unit IV – Equilibrium Thermodynamics:**

Laws of Thermodynamics, Thermodynamic functions (U, H, S, G, and A) - Maxwell relationstemperature and pressure effects. Chemical equilibrium – Le Chatelier's Principle - equilibrium constant.

#### Unit V – Phase Transformation and Phase diagram:

Phase rule, Phase stability, thermodynamics of phase transitions, simple mixtures, colligative properties, Phase diagrams: One and Two-component systems - azeotropes, eutectics, congruent and incongruent melting.

#### **Textbook:**

- 1. A. G. Sharpe, Inorganic Chemistry, 3<sup>rd</sup> Edition, Addison-Wesley, 1999.
- 2. J. D. Lee, A New Concise Inorganic Chemistry, 3<sup>rd</sup> Edition., ELBS, 1987.
- 3. D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, ELBS. 1990.
- 4. Organic Chemistry, P. Y. Bruice, Pearson Education, 7<sup>th</sup> Edn, 2013.
- 5. P. Atkins, J. de Paula, J. Keeler, Physical Chemistry, 11<sup>th</sup> Edition, Oxford University Press, Oxford, United Kingdom, 2018.
- 6. D. A. McQuarrie & J. D. Simon, Physical Chemistry: A Molecular Approach, University Science Books, CA, 1997.

#### CHEM 2102 General Chemistry IV

**Learning** This course explores the basic treatment of halogen and noble gases, and **Objectives:** stereochemistry and chemistry of aromatic hydrocarbons. It also covers the electrochemistry part of equilibrium thermodynamics and solve the one-electron problem quantum mechanically.

Learning The students may understand and write mechanisms and stereochemical effects on various chemical reactions. Able to understand the electrochemical reactions in thermodynamic perspective and get insight of solving the wave equation for one-electron problem.

#### **Course Content:**

#### Unit I – Halogens and Noble Gases (Basic treatment):

Introduction; hydrogen halides; general considerations of halides; pseudohalogens; interhalogen compounds and polyhalogeno ions; oxides and oxyfluorides of Cl, Br and I; oxo- acids of halogens and their salts; aqueous solution chemistry; organic derivatives. Noble gases: Introduction; compounds of Xe, Kr and Rn; Chemical properties, structure and bonding.

#### **Unit II – Stereochemistry:**

Chirality – optical activity – central chirality, axial chirality, planar chirality, helicity, achiral diastereomers, prochirality, other stereochemical descriptors; configurational nomenclature (R/S) – CIP rule. Selectivity in organic reactions, configurational and conformational effects on reactivity. Source of chiral molecules – resolution and asymmetric synthesis (basic treatment).

#### **Unit III – Chemistry of Aromatic Hydrocarbons:**

Aromaticity, Huckel rule, annulene, benzenoid, nonbenzenoid, heteroaromatics, charged aromatics, fulvenes, fulvalenes, anti-aromatics and homoaromatics, structure and reactions of benzene, activity and orientation of substituted benzenes. Introduction to other aromatic systems.

#### **Unit IV – Electrochemistry:**

Electrochemical cells, half-cell potentials and cell potentials, determination of activities and activity coefficients of electrolytes- Debye-Hückel limiting law -Thermodynamic information from electrochemistry- Nernst equation - Electrode potentials.

#### **Unit V – Solving One-electron Atom:**

The Schrödinger equation – Atomic units – Relative coordinates - spherical polar coordinates – Separation of variables – Angular part – The Radial equation and its simplification – Asymptotic solution for  $\rho$  equation – Laguerre and associated Laguerre polynomials – Origin of quantization of solutions – Interdependency between quantum numbers.

#### **Textbooks:**

- 1. Organic Chemistry, P. Y. Bruice, Pearson Education, 7<sup>th</sup> Edn, 2013
- 2. E. L. Eliel, Stereochemistry of Carbon Compounds. John Wiley (1997)
- 3. A. G. Sharpe, Inorganic Chemistry, 3<sup>rd</sup> Edition, Addison-Wesley, 1999.
- 4. J. D. Lee, A New Concise Inorganic Chemistry, 3<sup>rd</sup> Edition., ELBS, 1987.
- 5. P. Atkins, J. de Paula, J. Keeler, Physical Chemistry, 11<sup>th</sup> Edition, Oxford University Press, Oxford, United Kingdom, 2018.
- 6. D. A. McQuarrie & J. D. Simon, Physical Chemistry: A Molecular Approach, University Science Books, CA, 1997.
- 7. I. N. Levine, Quantum Chemistry, 7<sup>th</sup> Edition, Pearson Education, Inc. NJ, 2014.

#### **CHEM 2201 Inorganic Chemistry I**

**Learning** Study of p-block elements and their compounds provides a strong foundation to the understanding of periodic properties of elements and this course provides an opportunity to study periodic properties.

Learning Students after completing will be able to predict various reactions of elements and their synthetic methodology.

#### **Course Content:**

#### Unit I – Acids and Bases:

Bronsted acids and bases: Bronsted acidy, periodic trends in Bronsted acidy, Lewis acids and bases: definitions, adduct formation, strengths, stability; super acids; HSAB principle and its applications.

#### **Unit II – Solid State Chemistry:**

Inorganic Solids: Ionic solids, close packing, radius ratio, ionic radii, lattice energy; crystal structure, cubic systems (SC, BCC, FCC), fluorite, antifluorite, zincblende, rutile; defects in ionic solids; insulators, semiconductors, and superconductivity.

#### **Unit III – Early Transition Elements:**

Introduction and the chemistry of Scandium group, Titanium group, Vanadium group, Chromium group and Manganese group.

#### **Unit IV – Late Transition Elements**:

Introduction and the chemistry of Iron group, Cobalt group, Nickel group, Copper group and Zinc group.

#### Unit V – Nuclear Chemistry- Basic Treatment:

Introduction; nuclear binding energy; radio-activity and nuclear reactions; nuclear fission and fusion; spectroscopic techniques based on nuclear properties; separation of stable isotopes and unstable isotopes; applications of isotopes.

#### **Text Book:**

- 1. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2<sup>nd</sup> Edn, BH, 1997
- 2. K. F. Purcell and J. C. Kotz, Inorganic Chemistry, 2<sup>nd</sup> Edn, Cengage Learning, 2012
- 3. F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 6<sup>th</sup> Edn, John Wiley, 2004.
- 4. D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, ELBS. 1990.
- 5. A. G. Sharpe, Inorganic Chemistry, 3<sup>rd</sup> Edn, Addison-Wesley, 1999.
- 6. J. D. Lee, A New Concise Inorganic Chemistry, 3<sup>rd</sup> Edn, ELBS, 1987.
- 7. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3<sup>rd</sup> Edn, John Wiley, 2001.
- 8. L. Jolly, Modern Inorganic Chemistry, 2<sup>nd</sup> Edn, McGraw-Hill, 1991.
# **CHEM 2202 Organic Chemistry I: Functional Group Transformations**

Learning	Reactions	of	functional	groups	attached	with	sp <sup>3</sup> ,	sp <sup>2</sup>	and	sp	carbons.
<b>Objectives:</b>	Understani	ding	g these proce	esses with	help of ba	asic or	ganic	react	ion m	echa	nism.

Learning Identify the nucleophile, electrophile and free radical and their reactivity pattern.Outcome: Identify the oxidation states of carbon bearing functional groups. Transforming functional groups.

# **Course Content:**

# Unit I – Substitution and Elimination Reactions:

Identifying and generating nucleophiles and electrophiles. Types of reactions, mechanism of reactions. Substitution at saturated reaction center  $-S_N 1$ ,  $S_N 2$  and  $S_N i$  mechanism - stereochemical outcome of the products; elimination reactions-generating carbon – carbon and carbon – heteroatom multiple bonds – E1, E2, E1cB.

# **Unit II – Electrophilic Substitution Reactions:**

Aromatic electrophilic substitution reactions – o-, m-, p- directing groups, manipulation of aromatic compounds using substitution reactions, aromatic nucleophilic substitution reactions. Benzyne generation and reactivity.

# **Unit III – Reactions of Electrophilic Unsaturated Carbons 1:**

Generation and reactions of carbon heteroatom multiple bonds (C=O, C=N, C=N bonds), addition reactions to carbon heteroatom multiple bond, addition – elimination reactions of carbon heteroatom multiple bond. Selected reduction reactions of carbon heteroatom multiple bonds.

#### **Unit IV – Reactions of Electrophilic Unsaturated Carbons 2:**

Substitution reactions at  $\alpha$ -carbon of carbon heteroatom multiple bonds – enolate chemistry. Reactions of  $\alpha$ , $\beta$ -unsaturated carbonyl compounds – addition reactions.

# **Unit V – Rearrangement Reactions:**

Rearrangement reactions (anionic, cationic and free radical); examples of different kind of rearrangements.

- 1. Organic Chemistry, P. Y. Bruice, Pearson Education, 7<sup>th</sup> Edn, 2013
- 2. Organic Chemistry: An Acid-Base Approach, M. B. Smith, CRC Press, 3<sup>rd</sup> Edn, 2022.
- 3. Organic Chemistry as Second Language, D. R Klein, 2004, John Wiley and Sons, USA.
- Organic Chemistry, W. H. Brown, C. S. Foote, B. L. Iverson and E. V. Anslyn, Brooks/Cole Cengage Learning, 6<sup>th</sup> Edn, 2012.
- 5. Organic Chemistry, Clayden, Greeves, Warren, Oxford University Press, 2<sup>nd</sup> Edn, 2012.
- 6. Principles of Organic Synthesis, R.O.C. Norman and J. M. Coxon, 3<sup>rd</sup> Edn, 1994.
- 7. F. A. Carey and R. J. Sundberg (Part A and B) Kluwer Academic / Plenum Publishers (2000).

# CHEM 2203 Physical Chemistry I

- Learning Students will learn fundamentals of group theory, molecular symmetry and its applications to the chemical systems. This physical chemistry course covers microscopic aspects of thermodynamics at molecular level in statistical perspective. The relation between the microscopic to the macroscopic systems is provided and applications aspects of electrochemistry
- Learning The student will acquire knowledge to understand the molecules in symmetry outcome:aspects and also get insights of statistical aspects of molecule and able to measure the electroanalytical parameters through electroanalytical techniques.

# **Course Content:**

# Unit I - Group Theoretic Exploration of Molecular Symmetry

Definition and Properties of Group – Subgroups – Classes - Symmetry elements and Operations – Products of symmetry Operations – Equivalence of Symmetry elements and atoms – Relationship among Symmetry elements and operations – Schoenflies Point Groups – Point groups with multiple higher-order axes – flowchart for Point group assignment- Chirality, Dipole moment and other Consequences of symmetry.

# **Unit II – Molecular Symmetry Groups and Matrices**

Matrix representation of symmetry Operations and its Character – Classes of symmetry operations – The Great Orthogonality Theorem (without proof) – Construction and Usage of Character tables – Reducible and Irreducible representations – Symmetry Adapted Linear Combinations - Projection operators – Direct Products.

# **Unit III – Statistical Thermodynamics:**

The Boltzmann distribution – Molecular Partition functions and thermodynamic properties – Molecular energies - translational, rotational, vibrational, electronic contributions – Ensembles – Averaging Postulates – Mean energy and its variation – Calculations for model systems.

# **Unit IV– Kinetic Theory of Gases:**

Macroscopic and microscopic states, model system of a dilute gas, velocity probability distribution, distribution of molecular speeds, root mean speed, pressure of dilute gas, effusion and wall collisions, system with potential energy: intermolecular forces, hard sphere gas, Fick's Law, diffusion, thermal conductivity, viscosity of gases.

# **Unit V – Electrochemistry-Applications:**

Ionic equilibrium– electrolysis – cyclic voltammetry– potentiometric titration– conductometric titration – Kohlrausch law– electrical double layer.

- 1. F. Albert Cotton, Chemical Applications of Group Theory, 3<sup>rd</sup> Edition, Wiley, 1990.
- 2. P. Atkins, J. de Paula, J. Keeler, Physical Chemistry, 11<sup>th</sup> Edition, Oxford University Press, Oxford, United Kingdom, 2018.
- 3. T. Engel, P. Reid, W. Hehre, Physical Chemistry, 3<sup>rd</sup> Edition, 2013.
- 4. D. A. McQuarrie & J. D. Simon, Physical Chemistry, I<sup>st</sup> Edition, University Science, 1997.
- 5. E. V. Anslyn & D. A. Dougherty, Modern Physical Organic Chemistry, University Science, 2004.

# CHEM 3101 Inorganic Chemistry II: Chemistry of Transition Metal Complexes

Learning Objectives:	Course electron	describes nic properti	the es.	nature	of	coordination	complexes	and	their	struct	ures,
	~ .										

LearningStudents undergoing this course will have working knowledge on synthetic and<br/>analysis of coordination complexes and their involvement in biological systems.

# **Course Content:**

# **Unit I – Introduction to Transition Metal Complexes:**

A brief review of the general characteristics of transition elements, types of ligands, nomenclature of coordination complexes, chelates, chelate effect, geometry and isomerism, Werner, Sidzwick and Valence bond theory.

# **Unit II – Electronic Structure of Transition Metal Complexes 1:**

Crystal field theory, crystal field splitting, application of d-orbital splittings to explain magnetic properties, low spin and high spin complexes, crystal field stabilization energy, spectrochemical series, weak and strong field complexes, thermodynamic and related aspects of crystal fields, ionic radii, heats of ligation, lattice energies, site preference energies.

# **Unit III – Electronic Structure of Transition Metal Complexes 2:**

MO theory of complexes (quantitative principles involved in complexes with no pi and with pi bonding) and ligand filed theories and molecular symmetry, angular overlap model, Jahn Teller effect, electronic spectra of transition metal complexes, Orgel and Tanabe-Sugano diagrams, charge transfer and d-d transitions, nephelauxetic series.

# **Unit IV – Inorganic Reaction Mechanisms:**

Inert and labile compounds, substitution reactions of octahedral complexes, dissociative, associative, aquation, conjugate base mechanism; substitution reactions of square planar complexes, trans effect, trans effect series, theories of trans effect; electron transfer reactions.

# Unit V – Magnetism and Inner Transition Elements:

Magnetism: Types of magnetism – dia-, para-, ferro- and antiferromagnetism, quenching of orbital angular moment, spin-orbit coupling – Faraday balance, Guoy balance, SQUID, VSM.

Chemistry of lanthanides and actinides: lanthanide contraction, oxidation states, spectral and magnetic properties, use of lanthanide compounds as shift reagents.

- 1. D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, 3<sup>rd</sup> Edn. ELBS. 1999.
- 2. J. E. Huheey, Inorganic Chemistry, 4<sup>th</sup> Edn., Harper International.
- 3. F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 5<sup>th</sup> Edn., John Wiley.
- 4. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3<sup>rd</sup> Edn., John Wiley, 2001.
- 5. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2<sup>nd</sup> Edn., BH, 1997.
- 6. W. L. Jolly, Modern Inorganic Chemistry, 2<sup>nd</sup> Edn., McGraw-Hill, 1991.

# CHEM 3102 Organic Chemistry II: Synthetic Methods, Polymers and Spectroscopic Techniques

- **Learning** The functional group interconversions and C–C bond forming reactions. Synthesis and reactivity of aromatic heterocycles. Structural characterization of organic molecules.
- LearningConstructing organic molecules through C–C bond formation and functional group<br/>transformation. Recognize the cyclic transition states in organic reactions.<br/>Polymerization reactions. Structural characterization using spectroscopy.

# **Course Content:**

# Unit I – Name Reactions in Organic Synthesis:

Baylis-Hillman reaction, Bischler-Napieralski synthesis, Dieckmann condensation, Finkelstein reaction, Hell–Volhard–Zelinsky reaction, Kulinkovich reaction, Mannich reaction, McMurry coupling, Nef reaction, Pictet-Spengler reaction, Ugi reaction, Simmon-Smith cyclopropanation reaction, Yamaguchi macrocyclization, Wittig and related reactions.

# **Unit II – Pericyclic Reactions (Introductory Level):**

Concerted vs non-concerted pathways, types of pericyclic reactions – electrocyclic reactions (Con and Dis rotatory processes), cycloadditions - Diels-Alder (hetero, retro variants, normal and inverse electron demand), dipolar cycloaddition, sigmatropic reactions, – *supra* and *antra* facial shifts, ene reactions, cheletropic reactions.

# Unit III – Organometallics in Organic Synthesis:

Organometallic compounds - nomenclature, structure, reactivity, basicity – synthesis and applications of organolithium, organoboron, organocopper, organozinc, organomagnesium, organotin and organosilicon compounds in organic synthesis.

# **Unit IV – Introduction to Synthetic Polymers:**

General classes of synthetic polymers, chain growth polymers – living polymers, stereochemistry of polymerization, polymerization of dienes, co-polymers, step-growth polymers, physical properties of polymers, bio-degradable polymers.

# Unit V – Structural Characterization of Organic Compounds (Introductory Level):

Introductory level - UV- Visible spectroscopy, infrared spectroscopy, NMR spectroscopy and Mass spectrometry.

- Strategic Applications of Organic Named Reactions in Organic Synthesis, L. Kürti and B. Czakó, Elsevier Academic Press, 2005.
- 2. Organic Chemistry, Clayden, Greeves, Warren, Oxford University Press, 2<sup>nd</sup> Edn, 2012.
- 3. Principles of Organic Synthesis, R.O.C. Norman and J. M. Coxon, Chapman & Hall, 3<sup>rd</sup> Edn, 2001.
- 4. Introduction to Organic Chemistry, C. H. Heathcock, A. Streitweiser and K. M. Kosower, Medtech, 4<sup>th</sup> Edn, 2017.
- 5. Organic Chemistry, P. Y. Bruice, Pearson Education, 7<sup>th</sup> Edn, 2013.
- 6. F. W. Billmeyer, Textbook of Polymer Science, Wiley-India, 2007.

# CHEM 3103 Physical Chemistry II – Reaction Kinetics

Learning Objectives:	Knowledge about speed of the reaction and its dependence on various variables gives an insight to understand mechanisms of reactions in kinetic aspects.
Loomina	A ften completing this course, students meruna denotes of the linetics of different types

LearningAfter completing this course, students may understand the kinetics of different typesOutcome:of reactions and understands kinetics of surfaces and catalysis.

### **Course Content:**

# **Unit I – Free Energy Relationships:**

Review of Rate law, Rate constants and order – Free energy of activation – Linear Gibbs energy relations – Edward's Equation and alpha effect – Theories of Acids and bases – Equilibrium constant – kinetic effects – Thermodynamic and kinetic control of reactions. Hammond postulate, Curtin-Hammett principle – Hammett equation and its applications.

# **Unit II – Reaction Dynamics:**

Collision theory – Lindemann-Hinshelwood and RRKM model – Diffusion control – Molecular Beams & collisions - Transition state theory – Eyring equation – Barrierless reactions - Activated complex – Arrhenius equation - kinetic isotope effect – Kramer's theory -Statistical approach to TS – PES of Excited states – Conical Intersections & avoided crossings – Spin-orbit coupling – branching and seam spaces.

# Unit III – Photo & Fast Reactions:

Photo physics of Unimolecular processes – Delayed fluorescence – Kinetics of bimolecular processes – Collision quenching – Stern-Volmer relations – Concentration dependence of quenching – Excimers – electron transfer in Excited state – Exciplex, Twisted intramolecular charge transfer processes - proton couple electron transfer processes – Features of fast reactions – study by flow method – relaxation methods – Flash photolysis.

# Unit IV – Kinetics of Surfaces and Catalysis:

Solid surfaces and its growth – Physisorption and Chemisorption – Adsorption and Desorption – Adsorption isotherms – Rate and extent of adsorption and desorption – Experimental assessment – molecular picture of adsorption and mobility – Catalysis – General Principles – Heterogenous and Homogenous catalysis – Catalysts and its types – Mechanisms – Catalytic cycles – enzyme kinetics.

# Unit V – Kinetics of Electron transfer and Electrodes:

Electron transfer in homogenous systems - rate law and rate constant – tunnelling –reorganization – Markus-Hush theory - Electrical Double layer – Electrode solution interface - Butler–Volmer equation – Tafel Plots – Voltammetry – Cyclic voltammetry and its applications – Electrolysis – working Principles of Galvanic cells – Nature of Electrochemical reactions – Mechanistic elucidation of electrode reactions.

#### **Textbook:**

- 1. P. W Atkins & J. D. Paula, Physical Chemistry, 10<sup>th</sup> Edition, W. H. Freeman & co.
- 2. T. Engel, P. Reid, W. Hehre, Physical Chemistry, 3<sup>rd</sup> Edition,
- 3. D. A. McQuarrie & J. D. Simon, Physical Chemistry, Ist Edition, University Science.
- 4. E. V. Anslyn & D. A. Dougherty, Modern Physical Organic Chemistry, University Science.

Credit: 4

### CHEM 3100 Summer Internship and Review Writing

Learning
Objectives
and
Outcome:
Students are encouraged to visit other research establishments to understand work culture. They are expected to learn to integrate chemistry to other domains of sciences, industrial research, and other related fields. The students acquire the skill of identifying a new research project, analyze, and submit for possible external funding.

Learning<br/>Plan and<br/>AssessmentStudents submit a report in the DST-style on the knowledge gained during their<br/>summer internships. The submitted report will be validated and analyzed by group<br/>of experts and award grade

# CHEM 3201 Inorganic Chemistry – III: Organometallics and Bioinorganic Chemistry

LearningTo learn about the nature of organometallic compounds, synthesis, characterizationObjectives:and catalytic applications and to learn essentials of bioinorganic chemistry.

Learning Successful completion of this course will make students to relate organometallic based on metal systems and their applications. Additionally, student may appreciate the relevance of inorganic systems in biology with reference to their structures and electronic properties.

# **Course Content:**

### Unit I – Organometallic Chemistry 1:

Compounds with transition metal to carbon bonds: classification of ligands, nomenclature, eighteen electron rule; transition metal carbonyls: range of compounds and structure, bonding, vibrational spectra, preparation, reactions; transition metal organometallics: square planar complexes, metal alkyls, metal alkylidenes, and metal alkylidynes; Structure and bonding: metal-olefin bond and arene metal bond.

### **Unit II – Organometallic Chemistry 2:**

Compounds with ligands having extended pi systems: bis(cyclopentadienyl) compounds, cyclopentadienyl carbonyl compounds, bis(arene) compounds, arene carbonyl compounds; isolobal analogy, metal-metal bond, transition metal clusters; clusters and catalysis; hydride and dihydrogen complexes; fluxionality.

### **Unit III – Organometallic Chemistry 3:**

Organometallic reactions and catalysis: oxidative addition, reductive elimination, insertion, hydride elimination, abstraction; olefin hydrogenation, hydroformylation, Wacker process, Ziegler-Natta polymerisation, cyclo oligomerisation, olefin isomerisation, olefin metathesis, Monsanto acetic acid synthesis, Fischer-Tropsch process, hydrosilylation.

#### **Unit IV – Bioinorganic Chemistry 1:**

Metal ions in biological systems: heme proteins, hemoglobin, myoglobin, hemerythrin, hemocyanin, ferritin, transferrin, siderophores, cytochromes. Iron-sulphur proteins: rubredoxin, ferredoxin and model systems.

#### Unit V – Bioinorganic Chemistry 2:

Metalloenzymes: active sites, carboxy peptidase, carbonic anhydrase, superoxide dismutase, catalase, peroxidase, vitamin  $B_{12}$ , photosynthesis, nitrogen fixation, nitrogenase;  $Na^+/K^+$  ion pump, ionophores, metallodrugs, metal-nucleic acid interaction.

- 1. P. Powell, Principles of Organometallic Chemistry, 2<sup>nd</sup> Edn., ELBS, 1991.
- 2. K. F. Purcell and J. C. Kotz, Inorganic Chemistry, 2<sup>nd</sup> Edn., Cengage learning, 2012.
- 3. E. Huheey, Inorganic Chemistry, 4<sup>th</sup> Edn., Harper International, 2001.
- 4. C. Elschenbroich, A. Salzer, 2<sup>nd</sup> Edn., VCH, 1992.
- 5. F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 5<sup>th</sup> Edn., John Wiley.
- 6. R. W. Hay, Bio-Inorganic Chemistry, Ellis Horwood, 1987.
- 7. Lehninger, Principles of Biochemistry, Van Eikeren, 1982.
- 8. T. M. Loehr, Iron carriers and Iron proteins, VCH, 1989.
- 9. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books, CA, 1994.

# CHEM 3202 Organic Chemistry III: Heterocycles, Biomolecules and Drugs

Learning Objectives:	Effect of replacing carbon/s by heteroatom/s on properties of aromatic hydrocarbons. The functional group transformations. Basics about drug molecules.
Learning Outcome:	Application of functional group transformations in synthesis of heteroaromatics. Recognizing the structure and chemistry of biomolecules. Molecular interaction with drug target (biomolecules).

# **Course Content:**

# Unit I – Chemistry of Aromatic Heterocyclic Compounds:

Structure, synthesis and reactivity of five and six – membered aromatic heterocycles with one hetero atom and benzo-fused hetero-aromatics with one/two heteroatoms.

# Unit II – Chemistry of Carbohydrates and Lipids:

Classification of carbohydrates, the D and L notation, chemistry of monosaccharides, formation of glycosides, the anomeric effect, reducing and non-reducing sugars, disaccharides, polysaccharides. Introduction to lipids – wax, fatty acids, phospholipids, prostaglandins, fat soluble vitamins, terpenes and steroids.

# Unit III – Amino acids, Peptides and Proteins:

Classification and nomenclature of amino acids, acid–base properties of amino acids, peptide bonds and disulfide bonds, introduction to protein structure: primary structure, how to determine the primary structure of a polypeptide or a protein, secondary structure, tertiary structure, quaternary structure, protein denaturation. Synthesis of amino acids, resolution of racemic amino acids; peptide synthesis – protection and deprotection of amino acids.

# Unit IV – Nucleosides, Nucleotides and Nucleic Acids:

Purine and pyrimidine bases, nucleosides and nucleotides, nucleic acids – DNA and RNA, helical forms of DNA.

# Unit V – Introduction to Organic Chemistry of Drugs:

Pharmacophores, classification of drugs, naming drugs, lead compounds, molecular modification, random screening, serendipity in drug development, receptors, drugs as enzyme inhibitors, QSAR.

- 1. Organic Chemistry, P. Y. Bruice, Pearson Education, 7<sup>th</sup> Edn, 2013.
- 2. Organic Chemistry, L. G. Wade and J. W. Simek, 9<sup>th</sup> Edn, Pearson, 2019.
- 3. Heterocyclic Chemistry at a Glance, J. A. Joule and K. Mills, Blackwell Publishers, 2007, USA.
- 4. Heterocyclic Chemistry, Thomas L. Gilchrist, Pearson Education, 3<sup>rd</sup> Edn, 2005, India.
- Organic Chemistry, W. H. Brown, C. S. Foote, B. L. Iverson and E. V. Anslyn, Brooks/Cole Cengage Learning, 6<sup>th</sup> Edn, 2012.
- 6. Lehninger Principles of Biochemistry, D. L. Nelson and M. M. Cox, 7<sup>th</sup> Edn., W. H. Freeman, NY, USA.

## CHEM 3203 Physical Chemistry III: Atomic Structure and Bonding

Learning	Predict the nature of bond and its properties through various Electronic structural
<b>Objectives:</b>	methods, bonding models, and intermolecular interactions

LearningTo develop conceptual knowledge about the electronic structure of atom, groundOutcome:and excited states, chemical bonding and molecular orbital theories.

### **Course Content:**

# Unit I – Approximation Methods for Many-electron Schrodinger Equation:

Atomic Hamiltonian – Independent Electron Model – Theory of Perturbation – Non-degenerate Perturbation theory – I & II Order Corrections – Perturbation Treatment of He – Degenerate Perturbation – Theory of Variation – Linear and non-linear Variation – Matrix formulation of Linear Variation – Secular Determinant – Variational treatment of He.

#### **Unit II – Electronic Structure of Multi-electron Atoms:**

Quantum Particles Indistinguishability – Electron Spin and its interpretations – Pauli's Antisymmetry principle – Excited states of Helium - Slater Determinants – Slater Type Orbitals – Mean Field approximation – Hartree and Hartree Fock SCF approximation – Aufbau principle – Spin-Orbit Coupling – Term Symbols – Hund's Rules – Deconstruction of Periodic table.

### **Unit III – Methods for Molecular Schrodinger Equation:**

Bonn-Oppenheimer Approximation – Electronic structure of H2+ - Numerical solutions – Valence Bond Theory – Nature of Exchange - Ground and Excited states of H2 – LCAO-MO Theory of ground and excited states of H2 – Comparison of VB and MO theories - Configuration interaction - HF-SCF Theory – Correlation.

#### **Unit IV – Theories of Chemical Bonding:**

Molecular orbitals of Homo and Hetero Diatomics – Orbitals Interaction Diagrams - Bonds & Lonepairs vs MOs – Bond order - sp Mixing and Avoided Crossing - MO Configuration – Electronic States and Term Symbols – Hybridization theory of valence atomic orbitals – Isovalent hybridization – VSEPR theory – Advantages and Limitations of bonding theories.

#### **Unit V – Orbital Interactions in Molecules:**

The simple Huckel method – Assumptions – Determinant, Energies and Wave functions – LCAO approximation –Total energies – Conjugation – Aromaticity – Population Analysis – Extended Huckel Theory – Symmetry and Overlap – Principles of FMO Interactions and Walsh diagrams – Hyperconjugation – Jahn-Teller effects – Cluster Bonding.

- 1. Ira. N. Levine, Quantum Chemistry, 7<sup>th</sup> Edition, Prentice Hall.
- 2. D. J. Griffiths, Introduction to Quantum mechanics, 2<sup>nd</sup> Edition.
- 3. J. P. Lowe & K. A. Peterson, Quantum Chemistry, 2<sup>nd</sup> Edition, Elsevier Academic.
- 4. P. W Atkins & R. S. Friedman: Molecular Quantum Mechanics, 4<sup>th</sup> Edition, Oxford.
- 5. D. A. McQuarrie, Quantum Chemistry, 2<sup>nd</sup> Edition, Pearson.

### CHEM 3204 Topics in Analytical Chemistry

- **Learning Objectives:** The aims are to provide a sound physical understanding of the principles of analytical chemistry and to show how these principles are applied in chemistry and related disciplines— especially in life sciences and environmental science.
- LearningStudents will be able to develop analytical methods and perform chemometricOutcome:analysis to understand the diverse aspects of analytical applications.

# **Course Content:**

# **Unit I – Tools and Data Handling:**

Balances, burettes, volumetric flasks, pipettes, calibration of tools, sampling. Errors and Statistics: significant figures, rounding off, accuracy and precision, determinate and indeterminate errors, standard deviation, propagation of errors, confidence limit, test of significance, rejection of a result.

# **Unit II – Separation Techniques:**

Solvent Extraction: distribution Coefficient, distribution ratio, solvent extraction of metals, multiple batch extraction, counter-current distribution. - Chromatographic Techniques: classification, theory of chromatographic separation, distribution coefficient, retention, sorption, efficiency and resolution. -Column, ion exchange, paper, TLC & amp; HPTLC: techniques and application. - Gas Chromatography: retention time or volume, capacity ratio, partition coefficient, theoretical plate and number, separation efficiency and resolution, instrumentation and application.

### **Unit III – Spectroscopic Techniques:**

Electromagnetic radiation, absorption, and emission of radiation – instrumentation: sources, monochromators, detectors. - Flame spectrometry: flame emission, AAS, ICP, instrumentation and application. - Absorption spectrometry: UV-VIS, IR, instrumentation, techniques and applications.

#### **Unit IV – Thermal and Radiochemical Techniques:**

Thermogravimetry: instrumentation and techniques, TGA curves, DTA and DSC, applications. Radiochemical methods: decay reactions, growth of radioactivity, radiation detectors, tracer techniques.

#### **Unit V – Electroanalytical Techniques:**

Electrogravimetry, coulometry, voltammetry, polarography, conductometry, instrumentation, techniques and application.

- 1. D. C. Harris, Quantitative Chemical Analysis, 4<sup>th</sup> Edn., W. H. Freeman, 1995.
- 2. G. D. Christian & J. E. O'Reily, Instrumental Analysis, 2nd Edn., Allyn & amp; Balon, 1986.

# CHEM 4101 Inorganic Chemistry IV: Advanced Main group Chemistry and Inorganic Spectroscopy

Learning	To understand boron and silicon compounds with their polyhedral structures and
<b>Objectives:</b>	applications, inorganic ring systems. Various spectroscopic applications to inorganic
	compounds.
Learning	Students can resolve problems related to the structure and spectra of inorganic
Outcome:	compounds.

# **Course Content:**

### Unit I – Boron:

Synthesis, properties, bonding and structures of B2H6, Wades rule - structural features and styx codification of  $B_4H_{10}$ ,  $B_5H_9$ ,  $B_5H_{11}$ ,  $B_6H_{10}$ ,  $B_{10}H_{14}$ , carboranes and their anions, metalloboranes, metallacarboranes, Borazine, Boron nitride, 11B NMR of boron compounds of this unit.

# Unit II – Silicon:

Silanes, cyclosilanes, siloxanes, cyclic siloxanes, Silicon nitrides, Silyl amines, Silicatesclassification, diversity of silicate minerals, synthesis and applications of silicones, zeolites and ultramarines.

### Unit III – Nitrogen, Phosphorous, Sulphur:

Hydrides- $N_2H_4$ -conformations, oxides and oxy acids of nitrogen, phosphorous, sulfur; phosphazinessynthesis, structure, reactivity, applications; comparison with borazine; <sup>31</sup>P NMR of compounds of this unit. Sulfur-nitrogen compounds- $S_4N_4$ ,  $S_2N_2$ , (SN)<sub>x</sub>.

### **Unit IV – Spectroscopic Applications to Inorganic Compounds 1:**

NMR: Principle, chemical shift, multinuclear NMR (<sup>11</sup>B, <sup>15</sup>N, <sup>19</sup>F, <sup>27</sup>Al, <sup>29</sup>Si, <sup>31</sup>P) -Analysis of Selected examples: FPO(OH)<sub>2</sub>, F<sub>2</sub>PO(OH), PF<sub>3</sub>Cl<sub>2</sub>, PF<sub>2</sub>Cl<sub>3</sub>, P<sub>4</sub>S<sub>3</sub>, TiF<sub>4</sub>, TiF<sub>6</sub><sup>2-</sup>, NH<sub>3</sub>, NF<sub>3</sub>, CO<sub>2</sub> in water, ClF<sub>3</sub>, SF<sub>4</sub>; cis-trans isomers: N<sub>2</sub>F<sub>2</sub>, (PR<sub>3</sub>)<sub>2</sub>PtX<sub>2</sub>, literature examples. UV-Vis: Principle, molar extinction coefficient, types of electronic transition, isobestic point, Analysis of selected examples: differentiation of various isomers-ORD, CD, Cotton effect;  $[Co(NH_3)_5ONO]^{2+}$ ,  $[Co(NH_3)_5NO_2]^{2+}$ ; VO<sup>2+</sup>, NiR<sub>4</sub>Cl<sub>2</sub>, literature examples. IR: Principle, wavenumber, Analysis of common ions, bridged complexes, hydrogen bonding systems, structural determination of NSF<sub>3</sub>, (CH<sub>3</sub>)<sub>3</sub>SnCl, literature examples.

# **Unit V – Spectroscopic Applications to Inorganic Compounds 2:**

EPR: Principle, Hyperfine splitting, Zero-Field splitting, Kramers' degeneracy; Analysis of Selected examples: Hydrogen and methyl radicals, AlH<sub>3</sub> radical, NO<sub>2</sub>,  $[Cr(H_2O)_6]^{3+}$ ,  $[Mn(H_2O)_6]^{2+}$ ,  $[(NH_3)_5Co-O-O-Co(NH_3)_5]^{5+}$ , Bis-salicylaldimine copper(II) complex, literature examples. Mossbauer spectroscopy: Principle, Quadrupole interactions, isomer shift, recoil energy, doppler effect, applications to <sup>57</sup>Fe, <sup>119</sup>Sn, <sup>127</sup>I, <sup>197</sup>Au compounds, literature examples. Photoelectron Spectroscopy (PS): Principle, Binding energy, Ultraviolet photoelectron spectroscopy (UPS), X-ray photoelectron spectroscopy (XPS), ESCA, Identification of elements by PES, Auger peaks, Surface analysis, band structure by PES.

# **Textbooks:**

- 1. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2ed, BH, 1997
- 2. J. E. Huheey, Inorganic Chemistry, 4ed, Harper International, 2002.
- 3. Russel S. Drago, Physical Methods in Inorganic Chemistry, Litton Educational Publishing, 2017
- 4. Stephan Hüfner, Tadeusz Waldemar Huber, Photoelectron Spectroscopy, Principles and Applications, Stephan Hüfner, Tadeusz Waldemar Huber, Springer Publications, 2003
- 5. D. F. Shriver, P. W. Atkins, C. H. Langford, 3ed, Inorganic Chemistry, ELBS. 1999.
- 6. F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 6<sup>th</sup> Edn, John Wiley, 2004.

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# CHEM 4102 Organic Chemistry IV: Spectroscopic Identification of Organic Compounds

Learning Objectives:	To learn the basic principles of modern spectroscopy and characterization principles of organic molecules.
Learning Outcome:	Skill to interpret the spectra of organic molecules and deduce the molecular structures.

# **Course Content:**

### **Unit I – Introduction**

Application of UV-Visible and IR Spectroscopy to Organic Structure Elucidation: UV – Visible Spectroscopy: Basic principles, application of UV – Visible spectroscopy to organic structure elucidation, Woodward – Fisher rules, Solubility of organic solids, isosbestic point, ORD – CD to stereochemical assignments, Octant rule. IR – Spectroscopy – Basic principles, characteristic frequencies of common functional groups.

# **Unit II – Application of NMR Spectroscopy:**

Basic principles. Introduction to NMR techniques – CW and FT NMR techniques. <sup>1</sup>H NMR Spectral parameters – intensity, chemical shift, multiplicity, coupling constant, factors affecting. Analysis of first order and second – order spectra. Structure determination of organic compounds by <sup>1</sup>H NMR spectra.

# Unit III – Multinuclear NMR (with specific emphasis on <sup>13</sup>C NMR):

Proton coupled; off–resonance decoupled; proton noise decoupled <sup>13</sup>C NMR spectra. Assignment of chemical shifts, additively effect, characteristic chemical shifts of common organic compounds and functional groups, DEPT and SEFT spectra. NMR of common heteroatoms present in organic compounds (N, F, O, P, S and D) 2D NMR techniques  ${}^{1}\text{H} - {}^{1}\text{H} \text{ COSY}$ ,  ${}^{1}\text{H} - {}^{13}\text{C} \text{ COSY}$ , HMQC, HMBC, NOESY and INADEQUATE spectra

# Unit IV – Application of Mass Spectroscopy to Organic Structure Elucidation:

Basic principles, techniques of ion production, ion and daughter ions, molecular ion and isotope abundance, nitrogen rule, energetics of fragmentation - metastable ions, common fragmentation pathways – fragmentation pattern of common chemical classes.

# Unit V – Problem solving exercises involving UV, IR, NMR & MS data:

Problems involving interpretation of spectral details of organic compounds

# **Reference Books:**

- 1. R. M. Silverstein and F. X. Webster, Spectrometric identification of organic compounds., John Wiley and Sons. Inc., Sixth edition (1997).
- 2. W. Kemp, Organic Spectroscopy, Third Edition, MacMillon (1994).
- 3. Pavia, Lampman and Kriz, Introduction to Spectroscopy, 3<sup>rd</sup> Edn., Brooks/Cole Pubs. Co.
- 4. D. H Williams and Ian Fleming, Spectroscopic methods in organic chemistry, Tata McGraw Hill, (1998).
- 5. William Kemp, Introduction to multinuclear NMR.

# CHEM 4103 Physical Chemistry IV: Principles of Spectroscopy

**Learning** To develop a working knowledge in the theory of absorption and emission **Objectives:** spectroscopy from classical and quantum sciences.

**Learning** Familiar with probability of transition, selection rule. Simulate electromagnetic spectrum of simple molecules.

#### **Course Content:**

#### **Unit I – Electronic Spectra:**

Electromagnetic radiation – Interaction with matter – Electronic energy levels and CI - SALC – Absorption and Emission – Transition moments and probability – Selection rules – Intensities - Broadening – Vibronic transitions – Frank-Condon Principle – Vibrational progressions and excited state geometry – Radiative and Non-radiative decay - XPS & Auger electron spectra.

### **Unit II – Rotational and Vibrational Spectra:**

Pure Vibrational and Rotational spectra - Spectra of Di and Polyatomics - Normal Modes - Selection rules – Fermi Resonance – Anharmonicity and Isotope effect – Bond-lengths and strengths – Vibrational Localization of Functional groups – Polarizability and Raman effect - Rotational and Vib-Rotational Raman spectra – Fourier Transform - Exclusion Rule.

### Unit III – Magnetism and Magnetic Resonance:

Electrons and nuclei in magnetic field – Magnetic resonance spectroscopy – Nuclear magnetic resonance – Chemical shifts – Fine Structure – Conformational conversion and Exchange – Pulse Techniques – magnetization vector – spin relaxation and decoupling – NOE effect – 2D NMR – Electron paramagnetic resonance – g value – fine structure.

#### **Unit IV – Photochemistry:**

Photochemical Processes – Time-dependent Schrodinger equation & perturbation theory - Grothus-Draper and Stark-Einstein Laws – Jablonski Diagram for Excited States – Qualitative description of fluorescence, phosphorescence, and non-radiative processes – Quantum yield – Photosensitized processes – Energy Transfer processes – Two-photon absorption.

#### **Unit V – Solids and Diffraction methods:**

Close packing – FCC and HCP – Unit cells types – Bravais Lattices – Crystallographic Point and Space Groups – Miller Indices – Reciprocal lattice – Brillouin zone — XRD and Bragg's law – Lau, Debye-Scherrer, Bragg methods – Systematic Absences – Structure and Form Factors – Phase problem – Absolute configuration - Electron Diffraction and LEED.

- 1. Max Diem, Quantum Mechanical Foundations of Molecular Spectroscopy, Wiley-VCH, 2021.
- 2. Jeanne L. McHale, Molecular Spectroscopy, 2<sup>nd</sup> Edition, CRC Press, 2017
- 3. Hans Kuzmany, Solid State Spectroscopy. An Introduction, Springer, 2009
- 4. Ramakrishna V. Hosur, and Veera Mohana Rao Kakita, A Graduate course in NMR Spectroscopy, Springer, 2021

# CHEM 4201 Computational Chemistry

Learning Objectives:	Students learn how to use various computational software to find the equilibrium geometry of molecular systems and find various properties through simulations.
Learning	Student will be able to draw molecular structure, analyze eigen values, correlate eigen

#### **Course Content:**

**Outcome:** 

#### Unit I – Ab-initio Implementation of HF-SCF-MO theory:

values with physical properties.

Molecular Hamiltonian and Schrodinger equation – LCAO approximation – Effective Potential and Mean-Field Approximation – Antisymmetry and Slater determinant – Fock operator - Self-Consistent Field approximation – Roothan's equations - Density Matrix – Total energies – Koopman's theorem – Unrestricted and Restricted open shell HF – Spin contamination.

#### Unit II – Basis Sets:

Atomic Basis sets – Slater type orbitals – Split-valence – Gaussian Type Orbitals – Basis set Contraction – Polarization functions – Diffuse Functions – Popular Basis sets - Basis-Set superposition Error – Counterpoise correction – Basis set Extrapolation – Effective core potential – Computational issues.

#### **Unit III – Electron Correlation:**

Electron correlation – Static and Dynamic Origins – Density functional theory - Configuration Interaction (CI) – Configuration State Functions - CI matrix – Time complexity – Brillouin's theorem - Slater-Condon rules - Truncated CI – MRCI – MC SCF – CAS SCF — Moller-Plesset perturbation theory – Coupled Cluster Methods - Size Consistency and Extensivity.

#### **Unit IV – Characterization of Molecules:**

Equilibrium geometry – Potential energy Surface – Forces in Molecules – Hellmann-Feynmann Theorem – Characterization of Stationary points - Normal modes - Vibrational Analysis – Thermodynamic properties - Zero-point energy – Flowchart for Obtaining equilibrium geometry – Molecular Properties – Beyond Bonn-Oppenheimer approximation.

#### **Unit V – Practical Issues:**

Popular Electronic structure programs – Preparing the input - Choosing Methods and Basis sets – Interpreting the output file – Solving Convergence problems — Interpreting the imaginary frequencies – Use of direct products and Symmetry - Visualization of the Output - Illustrative examples – Population Analysis.

#### **Recommended Books:**

- 1. F. Jensen, Introduction to computational chemistry, Wiley, NY, 2007.
- 2. D. C. Young, Computational Chemistry, John-Wiley and Sons, NY, 2001.
- 3. C. J. Cramer, Essentials of Computational Chemistry, John-Wiley & Sons, 2004.
- 4. I. N. Levine, Quantum Chemistry, 7th edition, Prentice Hall.

# CHEM 4202 Manipulations of Organic Molecules

Learning Objectives:	To learn non-polar mechanism, constructing cyclic compounds, use of light and organometallic compounds in organic synthesis, functional group interconversions etc.
Learning	An integrated approach to manipulate any organic compound by observing and

Learning An integrated approach to manipulate any organic compound by observing and identifying their geometrical and electronic properties, participating functional groups, related theory, properties of reagents and catalysts, and other external variables.

### **Course Content:**

### **Unit I – Concerted Reactions:**

Cycloaddition, electrocyclic and sigmatropic and related pericyclic reactions - Explanations based on frontier orbital, Woodward-Hoffman and Huckel-Mobius theories - Application of concerted reactions in organic synthesis.

### **Unit II – Organic Photochemistry:**

Introduction to organic photochemistry - energetics of excitation - photochemistry of alkene, diene, aromatic, carbonyl and conjugated systems - Application of photochemical reactions in organic synthesis.

### Unit III – Modern Reagents in Organic Synthesis:

Introductory treatment to the application of silicon, phosphorus, selenium, palladium, ruthenium, rhodium, indium, titanium and samarium reagents in organic synthesis.

#### Unit IV – Rearrangement reactions in Organic Synthesis:

Review of rearrangement reactions and their application in organic synthesis (emphasis on reactions rather than reactivity)

# Unit V – Oxidation and Reduction Reactions in Organic Synthesis:

Oxidation of organic compounds with reagents based on peroxides, peracids, ozone, osmium, chromium, ruthenium, silver, dimethyl sulfoxide, iodine, and selenium dioxide. Reduction of organic compounds with reagents based on alkali and alkaline earth metals, boron, aluminum, hydrogen, hydrazine, formic acid and dissolving metals.

- 1. I. Fleming, Molecular Orbitals and Organic Chemical Reactions, John Wiley & Sons Ltd, 2009
- 2. R.O.C. Norman and J. Coxon, Principles of Organic Synthesis ELBS, 1994.
- 3. Smith, Organic Synthesis McGraw-Hill, 1996.
- 4. J. D. Coyle, Organic Photochemistry Wiley, 1985.
- 5. Carruthers, Modern Methods in Organic Synthesis, Academic Press, 1989.
- 6. F. A. Carey and R. J. Sundberg (Part A and B) Kluwer Academic / Plenum Publishers (2000).

# CHEM 4203 Crystal Engineering and Solid-State Properties of Molecular Materials

Learning Objectives:	Understanding some solid-state properties, such as polymorphism, pharmaceutical co- crystals, and mechanical, electrical, and magnetic properties of molecular crystals, that are some of the hot areas of current-day research.
Learning Outcome:	Learners will be able to design crystals with desired properties using the crystal engineering approach.

# **Course Content:**

### Unit I – Crystal engineering and pharmaceutical co-crystals:

Crystal systems, space groups, point groups, supramolecular synthons - hetero synthons and homo synthons, co-crystals - pharmaceutical co-crystals, polymorphism.

### **Unit II – Mechanical Properties of Molecular Crystals:**

Elastic bending, plastic bending, shearing, thermo-salient effect, photo-salient effect

### **Unit III- Thermal Expansion of Molecular Materials:**

Thermal expansion coefficients, Principal axes of thermal expansion, symmetry and thermal expansion, parameters influencing the thermal expansions

### **Unit IV–Introduction to Electrical Properties of Molecular Materials:**

Electrical conductivity in solids, dielectric materials, paraelectric materials, piezoelectric materials, pyroelectric materials, relaxation

#### Unit V–Introduction to Magnetic Properties of Molecular Materials:

Diamagnetic materials, paramagnetic materials, ferromagnetic materials, ferrimagnetic materials, antiferromagnetic materials

#### **Suggested Readings:**

- 1. G. R. Desiraju, J. J. Vittal and A. Ramanan, Crystal Engineering a Textbook, World Scientific Publishing Co. Pte. Ltd., 2011.
- 2. W. D. Callister, Jr. and D. G. Rethwisch, Fundamentals of Materials Science and Engineering an Integrated Approach, 5th edition, John Wiley & 2015.
- 3. K. Rissanen, Hot Topics in Crystal Engineering, Elsevier Inc, 2021.
- 4. R. Hilfiker, Polymorphism: in the Pharmaceutical Industry, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2006.
- 5. Crystal Engineering of Pharmaceutical Cocrystals in the Discovery and Development of Improved Drugs, Geetha Bolla, Bipul Sarma, and Ashwini K. Nangia, *Chem. Rev.* **2022**, *122*, 11514–11603.
- 6. From Molecules to Interactions to Crystal Engineering: Mechanical Properties of Organic Solids, Subhankar Saha, Manish Kumar Mishra, C. Malla Reddy, and Gautam R. Desiraju, *Acc. Chem. Res.* **2018**, *51*, 2957–2967.

# CHEM 4204 Asymmetric Synthesis

Learning	To learn the methods for making chiral molecules.
<b>Objectives:</b>	

**Learning** Able to explain the need for synthesizing biologically active compounds in optically pure form, the principles and strategies of making and analyzing enantio-enriched compounds.

# **Course Content:**

# Unit I – Introduction to Asymmetric Synthesis and Resolution:

Asymmetric synthesis importance and basic principles - stereoselective and stereospecific – enantioselective and diastereoselective. Energetic considerations, strategies for asymmetric synthesis – advantages and limitations of each strategy, analytical methods for determining enantiomeric excess. Resolution – resolving agents and resolution of racemic compounds having functional groups for eg. alcohol, amine, and acid. Resolution of chiral ligands – BINOL, trans-1,2-diaminocyclohexane. Kinetic resolution of racemic mixtures. Dynamic Kinetic resolution, enzymatic resolution.

### Unit II – Asymmetric Synthesis on Chiral Substrate:

Nucleophilic addition to  $\alpha$ -chiral carbonyl compounds; Prediction of stereochemistry – Cram's rule and related modifications. Double stereo differentiation; matched pair and mismatched pair; examples from aldol condensation and hydroboration reactions. Electrophilic addition to  $\alpha$ -chiral olefins – epoxidation, cyclopropanation, hydroboration – oxidation, alkylation of enolates of  $\beta$ -chiral carbonyl compounds.

### Unit III – Asymmetric Synthesis using Chiral Auxiliary:

Chiral auxiliary mediated reactions using various chiral auxiliaries. Chiral auxiliaries derived from proline, champhor, menthol and other chiral pool sources. SAMP/RAMP hydrazines and other pyrrolidines, oxithiane, oxazolidine-2-one, thiazolidine-2-one, phenylethylamine, 2-phenylcyclohexanol etc. Remote chiral Induction.

#### **Unit IV – Asymmetric Synthesis using Chiral Reagents:**

Chiral organoboranes – Application of chiral organoboranes, reduction (Ipc2BCl) and allylation and crotylation reactions. Chiral modification of lithium aluminum hydride, BINAL-H – application in reduction of prochiral ketones; oxazaborolidines.

#### Unit V – Asymmetric Synthesis using Chiral Catalysts:

Asymmetric alkylation and allylation of carbonyl compounds, reduction of ketones, imines. Asymmetric hydrogenation: early advances DIPAMP, DIOP and Noyori's BINAP selected reactions/examples. Sharpless epoxidation, dihydroxylation, aminohydroxylation of alkenes; Jacobson catalysts – Evans catalyst–aziridination. Nucleophilic addition, conjugate addition and cycloaddition reactions. Organocatalysis–proline mediated aldol reactions and further expansion in the field of organocatalysis. Organocascade reactions. Asymmetric Michael addition to  $\alpha$ ,  $\beta$ – unsaturated carbonyl compounds.

- 1. Asymmetric Synthesis, R. A. Aitken and S. N. Kilenyi, Springer Science Business Media, 1994.
- 2. Principles of Asymmetric Synthesis (Tetrahedron series in Organic Chemistry), R. E. Gawley, J Aube, Pergman, 1996.
- 3. Asymmetric Synthesis, G. Proctor, Oxford University Press, USA, 1997.

### **CHEM 4205 Polymer Science: Synthesis and Characterization**

**Learning** To describe the type of bond in a polymer and rationally design the monomers for a given polymer. To describe various methods used for synthesizing polymers. To use analytical methods to characterize a polymer. To study the properties of polymers.

**Learning** The learners will be able to design the monomers for the preparation of polymers of interest. The learners will be able to characterize and understand the properties polemers.

#### **Course Content:**

# **Unit I – Chain Polymerization:**

Free radical polymerization, Role of inihibitors and retarders, controlled radical polymerization – iniferters - atom transfer radical polymerization (ATRP) – nitroxy radical mediated (NMP) polymerization – reversible addition-fragmentation chain transfer (RAFT) polymerization. Anionic polymerization, co-ordination polymerization, Zieglar–Natta catalysts, single site catalysts, copolymerization, kinetics of polymerization and copolymerization.

### Unit II – Step and Miscellaneous Polymerization:

Polycondensation – role of functionality – cyclic vs. linear polymers, kinetics of polycondensation, different types of polymers made through step polymerization including Nylon 6,6. Electrochemical polymerization – metathesis polymerization – group transfer polymerization – enzyme-catalyzed polymerization.

### **Unit III – Polymerization Techniques and Polymer Processing:**

Bulk polymerization, solution polymerization, suspension polymerization, emulsion polymerization, interfacial polycondensation, solid and gas phase polymerization. Comparison of polymerization techniques. Compounding, calendaring, die casting, rotational casting, film casting, compression moulding, injection moulding, blow moulding, extrusion moulding, thermoforming, foaming, reinforcing, fiber spinning, electrospinning.

# **Unit IV – Molecular Weight of Polymers:**

Role of molecular weight on the properties of polymers, degree of polymerization, number average, weight average, sedimentation average and viscosity average molecular weights, polydispersity index and its significance, determination of molecular weight of polymers using cryoscopy, ebulliometry, membrane osmometry, vapor phase osmometry, end group analysis, viscometry, light scattering, ultracentrifugation, and gel permeation chromatography.

# **Unit V – Thermal Properties and Application of Polymers:**

Glass transition temperature (Tg) – factors influencing Tg – plasticizers – dilatometry, differential scanning calorimetry (DSC), thermomechanical analysis, dynamic mechanical analysis (DMA). Thermal stability of polymers – thermogravimetric analysis (TGA), differential thermal analysis (DTA). Conducting polymers – doping – synthesis and characterization of conducting polymers. Polymeric membranes for fuel cell applications, polymeric adhesives and sealants, rubbers vulcanization, use of rheometer in rubber industry, different types of synthetic rubber and their applications.

# **Reference Books:**

- 1. Fred W. Billmeyer, Textbook of Polymer Science, Wiley-India, 2007.
- 2. George G. Odian, Principles of polymerization, John Wiley and Sons, 2004.
- 3. Paul J. Flory, Principles of polymer chemistry, Cornell University Press, 1953.
- 4. V R Gowariker, N V Viswanathan, J. Sreedhar, Polymer Science, New Age International, 2003.

### CHEM 4206 Natural Products Chemistry

Learning	To create awareness about the various classes of natural products. To describe the
<b>Objectives:</b>	structural features of representative examples of each class of natural product.

**Learning** Can appreciate the chemical and biosynthetic way of synthesizing representative examples of each class of natural product.

#### **Course Content:**

### **Unit I – Chemistry of Terpenes:**

Biosynthesis of terpenoids – monoterpenes – sesquiterpenes – diterpenes (structure of terpenoids such as pinene, camphor, hirsutene, abietic acid, squalene etc).

#### **Unit II – Steroids:**

Biosynthesis of Steroids - Structure of common steroids such as cholesterol, ergosterol, stegmasterol, cholic acid – steroidal hormones; estrone, progesterone – testosterone – synthetic strategies towards steroids

### **Unit III – Polyphenolics and other Plant Coloring Molecules:**

Chemistry of flavones; isoflavones and aurones, biosynthesis and role of polyphenolics.

### **Unit IV – Alkaloids and Antibiotics:**

Biosynthesis and structure determination of representative examples of pyrrolidine, piperidine, indole, quinoline, and isoquinoline alkaloids; Structure of  $\beta$ -lactam antibiotics (penicillin)

#### **Unit V – Marine Natural Products:**

Introduction to marine natural products.

- 1. K. Nakanishi, Natural Product Chemistry Blackie Publications, 3 Vols.
- 2. R.H. Thomson, Chemistry of Natural Products Wiley, New York, 1996.
- 3. I.L. Finar, Advanced Organic Chemistry, ELBS, New Delhi, 1975.

# Credit: 4

# CHEM 4207 Supramolecular Chemistry

**Learning** Stabilization of chemical systems with non-conventional interactions and synthesis of materials with desired structures are challenging. This course aims to deal with these aspects.

**Learning** Students after completing this course may be able to design and synthesize new molecules with different shapes and geometry and explore their applications.

#### **Course Content:**

#### Unit I – Concepts of Supramolecular Chemistry:

Definition, Nature of supramolecular interactions, Host-guest interaction, Molecular recognition, Types of recognition, Self-assembly.

#### **Unit II – Cation-binding Hosts:**

Concepts, Cation receptors, Crown ethers, Cryptands, Spherands, Calixarenes, Selectivity of cation complexation, Macrocyclic and template effects.

#### Unit III – Binding of Anions and Neutral molecules:

Concepts, Anion host design, Anion receptors, Shape and selectivity, Neutral receptors, clathrates, cavitands, cyclodextrins, cyclophanes.

#### Unit IV – Applications of Supramolecular Chemistry:

Rational Design, Molecular Paneling, Supramolecular reactivity and catalysis, Supramolecular devices, Nanoscience applications.

#### Unit V – Supramolecular Chemistry in Biology:

Membranes, Macrocyclic systems, Photosynthesis, Oxygen transport, biological mimics, Enzymes, Metallobiosites, Heme analogues.

#### **Recommended Books:**

- 1. J. M. Lehn, Supramolecular Chemistry, Concepts and Perspectives, VCH, 1995.
- 2. H. Dodziuk, Introduction to Supramolecular Chemistry, Kluwer Academic, 2002.
- 3. F. Vogtle, Supramolecular Chemistry, An Introduction, John Wiley and Sons, 1991.
- 4. J. W. Steed, J. L. Atwood, Supramolecular Chemistry, A Concise Introduction, John Wiley, 2000.

# CHEM 4208 Bioinorganic Chemistry

**Learning** The course explains the role of metal ions in various biological processes and systems. **Objectives:** 

**Learning** After completing this course, students will understand the structural features of biological systems involving metal ions and their activities and mechanisms.

### **Course Content:**

### **Unit I – Introduction to Bioinorganic Chemistry:**

Introduction-Periodic survey of essential and trace elements- Biodistribution of metal ions-Biomolecules recap: sugars, amino acids, bioligands, peptides, proteins, enzymes, nucleosides, nucleotides, nucleic acids, cofactors, phospholipids-cell membrane and transport-active & amp; passive transport-symport, antiport, uniport, an ion pump, valinomycin, Gramicidin, enterobactin.

#### Unit II – Principles of Coordination Chemistry linked to Bio-inorganic Chemistry:

The link between Bio-inorganic and coordination chemistry- Thermodynamic aspects-hard-soft acid base concept-chelate effect-pKa value of ligands-tuning of redox potential-kinetic aspect-ligand exchange rate.

#### **Unit III – Metal-Protein Interaction, Metalloenzymes, and Biomimics:**

Metalloproteins, transport and storage proteins, Metalloenzymes- Classifications, metallohydrolases, Metallo oxidoreductases, Metallo isomerases, Metallo synthases, Metallolyases, Ligases, the role of metal ions in structural context - selected examples-Heme vs non-heme centers. Bioinorganic side of nucleic acid chemistry - Interactions with Metal Ions- Nuclease and Peptidase Models; Bioinspired metal complexes from recent literature.

### Unit IV – Physical Methods in Bioinorganic Chemistry:

Applications of spectroscopy for understanding biologically important molecules- Electronic spectra, vibrational spectroscopy, NMR, EPR, mossbauer spectroscopy, ORD, CD and MCD-Magnetic measurements-practical kinetics to biological systems.

#### **Unit V– Metallodrugs and applications:**

Metallodrugs – chelation in medicine-natural detoxification-Therapeutic Agents -cis-platin-Biochemical mechanisms of DNA damage-DNA repair-cancer treatment & cytotoxicity studies-Radiodiagnostic Agents- MRI Contrast Enhancement- insight into recent literature.

- 1. S.J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books, CA, 1994.
- 2. A. K. Das, Bioinorganic Chemistry, Arunabha Sen Publishers, 2016
- 3. Lehninger, Principles of Biochemistry, Van Eikeren, 1982.
- 4. K. D. Karlin and Z. Tyeklar, Bioinorganic chemistry of Copper, Chapman and Hall, Newyork, 1993.
- 5. W. P. Jencks, Catalysis in Chemistry and Enzymology, McGraw-Hill book company, 1969.
- 6. Robert A. Scott, Charles M. Lukehart, Applications of Physical Methods to Inorganic and Bioinorganic Chemistry, Wiley Publishers, 2007.

### CHEM 4209 Catalysis Concepts and Applications

Learning	To enable to students to understand the structure and properties and their relations of
<b>Objectives:</b>	metal complexes-based catalysts. The course also aims to give knowledge on various
	reaction mechanisms involving these types of catalysts.

LearningStudents after completing this course are equipped with designing metal complexesOutcome:with catalytic reactivity for various organic transformations.

### **Course Content:**

### **Unit I – Homogeneous Catalysis:**

Metal complex catalysis in the liquid phase –structure/activity relationships in homogeneous catalysis – steric effects– electronic effects of ligands, substrates, and solvents - catalyst recovery and recycling.

### Unit II – Heterogeneous Catalysis:

Classic gas/solid systems – the concept of the active site – model catalyst systems – real catalysts: promoters, modifiers, and poisons – surface organometallic chemistry – liquid/solid and liquid/liquid catalytic systems – aqueous biphasic catalysis – fluorous biphasic catalysis – biphasic catalysis using ionic liquids – phase-transfer catalysis – advanced process solutions using heterogeneous catalysis – the BP AVADA ethyl acetate process – the IFP and yellow diesel processes for biodiesel production.

### **Unit III – Industrial Process:**

Industrial process-ammonia synthesis (Haber-Bosch Technology), epoxidation catalysts, hydrogenation catalysts, the Shell Higher Olefins Process (SHOP), the Du Pont synthesis of adiponitrile, the Ciba–Geigy Metolachlor process. High- Fructose-Corn Syrup, the Mitsubishi Rayon acrylamide process, the BMS paclitaxel process, the Tosoh/DSM aspartame process.

#### Unit IV – Enzyme Catalysis:

The basics of enzymatic catalysis, active site and substrate binding models, common mechanisms in enzymatic catalysis, factors affect enzyme action-pH and enzyme function, temperature and enzyme function, applications of enzyme catalysis, binding enzymes to solid supports, replacing conventional routes with biocatalysis, developing new biocatalysts, abzymes, catalytic RNA.

# Unit V– Computer Applications in Catalysis Research:

Computers as research tools in catalysis – modeling of catalysts and catalytic cycles – a short overview of modeling methods – simplified model systems versus real reactions – modeling large catalyst systems using classical mechanics In-depth reaction modeling using quantum mechanics – predictive modeling and rational catalyst design.

# **Textbooks and References:**

- 1. G. Rothenberg, Catalysis: Concepts and Green Applications, Wiley-VCH, Weinheim.
- 2. Boy Cor, Wolfgang A. Hermann, Applied Homogeneous Catalysis with Organometallic Compounds, Vol.2, Wiley-VCH.
- 3. J. E. Huheey, E. A. Keiter R. L. Keiter and O. K. Medhi, Inorganic Chemistry: Principles of Structure and Reactivity, 4th Edn. Pearson Education Inc.
- 4. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, Advanced Inorganic Chemistry,5th Edn. John Wiley and Sons.
- 5. Warshel, A.; Sharma, P.K.; Kato, M.; Xiang, Y.; Liu, H.; Olsson, M.H.M. (2006). "Electrostatic Basis of Enzyme Catalysis". Chem. Rev. 106 (8): 3210-3235.

# CHEM 4210 Inorganic Photochemistry

**Learning** Course explains the reactions of coordination complexes in their photo-excited states. **Objectives:** 

**Learning** Students will be aware of various photo-physical and photo-chemical processes involved in coordination complexes.

### **Course Content:**

## **Unit I – Basic principles:**

Absorption of light –photochemical laws – photo stationary states – rate law – photolysis – quantum yields – actinometry – scavenging of reaction intermediates – flash photolysis – single photon techniques – flow techniques – picosecond transient kinetics.

### **Unit II – Kinetics of photoluminescence:**

Thermal effects of photoluminescence – luminescence yield – time resolved detection of excited states – radiative and non-radiative transitions – energy transfer.

### **Unit III – Photoredox reactions:**

Charge transfer complex – theory of electron transfer reactions – reactivity of CTTM, CTTL excited states – medium effects.

### **Unit IV – Ligand field photochemistry:**

General features of ligand field photochemistry – reaction of excited states of dn metal complexes.

# Unit V – Organometallic photochemistry:

Excited states in organometallic compounds – metal carbonyls – compounds with or without M-C bonds – hydride complexes.

#### **Recommended Books:**

- 1. K.K. Rohatgi-Mukherjee, Fundamentals of Photochemistry, Tata-McGraw Hill, 1981.
- 2. Collected readings in inorganic photochemistry, J. Chem. Edn. 1983
- 3. G. J. Ferraudi, Inorganic photochemistry, 1973
- 4. A.W. Adamson, E.D. Fleishcer, Concepts in inorganic photochemistry, 1963

# CHEM 4211 Ligand Field Theory

Learning	Understanding the bonding of coordination compounds will enable to develop materials												
<b>Objectives:</b>	with	important	properties.	This	course	deals	with	this	aspect	and	students	will	
	understand the nature to the bonding of ligands with metal ions.												

**Learning** Students, after completing this course, shall understand and interpret the electronic properties of metal complexes.

### **Course Content:**

#### **Unit I – Introduction:**

Qualitative basis of crystal fields, atomic spectroscopy (free ion, free ion terms, term wave functions, spin-orbit coupling), Thermodynamic aspects of crystal fields.

#### Unit II – Ions in Crystal Field:

Free ions in weak crystal fields (effect of a cubic crystal field on S, P, D, F, G, H, and I terms), Free ions in Medium and strong crystal fields.

#### **Unit III – MO theory of complex ions:**

Bonding in O<sub>h</sub>/T<sub>d</sub> complexes, qualitative calculations of 10Dq, Electronic spectra of complex ions.

### Unit IV – Magnetic properties of complex ions:

Complexes of non-cube stereochemistry, Actinide element compounds

#### **Unit V – ESR of complex ions:**

Theory and evaluation of spin Hamiltonian parameters for systems with s 1/2 and > 1/2.

- 1. B. N. Figgis, Introduction to Ligand Fields, Wiley Eastern Ltd., New Delhi/Bangalore, 1976.
- 2. A. B. P. Lever, Inorganic Electronic Spectroscopy, Elsevier, 1986.

# CHEM 4212 Miscellaneous Topics in Inorganic Chemistry

Learning Objectives: This course aims to comprehend the main group organometallic compounds, structure, and their properties. This course has an extensive view of the solid-state structures of inorganic systems including isopoly and heteropoly anions, spectral/magnetic properties of lanthanides and actinides and advanced levels of nuclear chemistry.
Learning Outcome: Students after completing this course will understand the main group organometallics and compare it with d-block organometallics. They can correlate various structures and may have knowledge in synthesizing materials with desired properties.

### **Course Content:**

### Unit I – Main group Organometallics:

Classification and structure, ionic and electron deficient compounds of groups 1, 2 and 12; Electron deficient compounds of the boron group; Electron-precise compounds of the carbon group. Electron-rich compounds of the nitrogen group.

### Unit II – Interhalogens, isopoly, and heteropoly compounds:

Pseudohalogens, Interhalogens, Xenon Compounds-Fluorides, oxides, oxyhalides- Poly oxo metallates-isopoly anions of Chromium, Vanadium, Phosphorous, Molybdenum and Tungsten, heteropoly anions of Molybdenum and Tungsten.

### Unit III – Lanthanides and Actinides:

Chemistry of lanthanides and actinides: lanthanide contraction, oxidation states, spectral and magnetic properties, use of lanthanide compounds as shift reagents.

#### **Unit IV – Inorganic Solids:**

Types of solids, covalent, ionic, molecular and metallic solids, Intermolecular forces in solids, close packed structures, CCP, HCP, Unit – cell, crystal lattices, radius ratio, lattice energy, Born-Lande equation, Born-Haber cycle for Lattice energy, Important examples for Perovskite-spinel-inverse spinel-rutile-Ilmenite structures- Imperfections in crystals- point defects, metal excess defect-F centers, metal deficiency defect.

### **Unit V – Nuclear Chemistry:**

Stability of nuclide, Radioactive decay and equilibrium, nuclear reactions, fission and fusion, nuclear reactor-basic component, Q value, cross sections, radioactive tracer techniques, neutron activation analysis, counting techniques such as G. M. ionization and proportional counter, Problems in nuclear chemistry.

- 1. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3ed, John Wiley, 2001.
- 2. H.J. Arnikar, Essentials of Nuclear Chemistry, 4ed, New Age Int. P. Ltd, 1995.
- 3. K. F. Purcell and J. C. Kotz, Inorganic Chemistry, 2ed, Cengage learning, 2012
- 4. F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 6ed, John Wiley, 2004.
- 5. J. E. Huheey, Inorganic Chemistry, 4ed, Harper International, 2002.
- 6. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2ed, BH, 1997S.K. Mehra, Advanced Nuclear Chemistry, Campus Books Internationals, 2009.

# CHEM 4213 Electroanalytical Techniques

**Learning** To enable students to use various electroanalytical methods to study and understand **Objectives:** corrosion and its mitigation, preparing energy storing materials, chemical reactivity

Learning Learners will be able to understand the fundamentals of electrochemistry and recogniseOutcome: the electrochemical processes, and various electroanalytical techniques.

# **Course Content:**

### **Unit I – Kinetics of Electrode Reactions:**

Mass transfer by Diffusion and Migration – models of electrode reactions – current potential characteristics – general mass transfer equation, migration and diffusion

### **Unit II – Potential Step Methods:**

Types of techniques, step under diffusion control, Ilkovic equation – polarographic analysis – sampled current voltammetry: reversible, irreversible processes, multicomponent systems

### **Unit III – Chrono Methods:**

Chronoamperometry, chronocoulometry – pulse polarographic methods: Tast pulse, normal pulse, differential pulse

#### **Unit IV – Potential Sweep Methods:**

Cyclic Voltammetry: Nernstian reversible, totally irreversible, quasi-reversible processes, multicomponent systems – convolute or semi-integral techniques

### **Unit V – Corrosion and Inhibition:**

Fundamentals: Corrosion Electrochemistry, electrochemical and local cell model of corrosion, Classification of corrosion, corrosion protection, measurement of wet corrosion, estimation of corrosion rate, Tafel plot, Linear polarization resistance, AC Impedance.

#### **Textbooks:**

- 1. J. Bard and L. R. Faulkner, Electrochemical Methods, Fundamentals and applications, John Wiley, 1980.
- 2. Bockris and Reddy, Electrochemistry, vol 1 and 2, Plenum, 1973.
- 3. H. Kissinger, Electroanalytical Techniques, John wiley, 1998

Credit: 4

## CHEM 4214 Molecular Reaction Dynamics

**Learning** Molecular reaction dynamics unfolds the history of change on the molecular level. It asks what happens on the atomic length and time scales as the chemical change occurs. The intention of this course is to describe why a particular experiment was carried out, what we have learned, what concepts are necessary to describe and understand the experiment, and how we move forward.

**Learning** Students can understand the bimolecular chemical reaction in gas phase and get insides into dynamic and mechanical aspects.

#### **Course Content:**

#### Unit I – Macroscopic and Microscopic Processes:

Introduction to molecular collisions – Collision parameters - From reaction cross-sections to rate coefficients – From microscopic dynamics to macroscopic kinetics

#### **Unit II – Potential Energy Surfaces:**

Two-body and three-body potentials energy functions – Reaction Path – Harpoon Mechanism – Steric Effect – Kinematic effect – Energy requirement for reactions with a barrier – Activated complex theory for rate coefficient - Transition state resonances - Activated complex theory for rate coefficient

### **Unit III – Molecular Energy Transfer:**

Simple models of energy transfer – State-to-state collisions – Bimolecular spectroscopy – Laser-assisted collision processes

### Unit IV – Reaction dynamics and Chemical reactivity:

Case studies: Bimolecular collisions – RRKM unimolecular reaction rate - Molecular dynamics of gas- surface reactions - van der Waals interactions on collisions

#### **Unit V – Simulations:**

Introduction to Molecular dynamics simulation package (classical and quantum mechanical treatment) – Case studies

- 1. Molecular Reaction Dynamics and Chemical Reactivity, R.D. Levine, R.B. Bernstein (Oxford, New York).
- 2. Theories of Molecular Reaction Dynamics the Microscopic Foundation of Chemical Kinetics, Niels Engholm Henriksen and Flemming Yssing Hansen, Oxford University Press, 2008

# CHEM 4215 Organic Synthesis for Chemical Biology – Principles and Practices

**Learning** Interdisciplinary approach in learning chemistry, application of organic chemistry in **Objectives:** the study of biological phenomenon. To equip the students with the principles and strategies of contemporary organic synthesis relevant to chemical biology applications.

**Learning** To be able to utilize the structure and function of organic molecules in biological system.

### **Course Content:**

### **Unit I – Chemical Biology:**

Chemical biology, origin, scope, academic and industrial perspectives, descriptors for biological relevance of an organic molecule, Lipinski rule, selected examples, challenges to synthetic chemists.

### **Unit II – Bioisosterism:**

Introduction – role of bioisosterism in drug development programs, classification of bioisostrism, effects of bioisosterism on biological activity, classical examples.

### **Unit III – Diversity Oriented Synthesis:**

Introduction - Diversity oriented synthesis – Principles and practices of DOS, substrate-based approach, reagent-based approach, Build / Couple / Pair strategy/sigma element, folding pathways / Classical examples from literature.

### **Unit IV – Multicomponent Reactions:**

Introduction — history of MCR, Classical MCRs Stecker, Mannich, Passereni, UGI, Hantsch/ Bignelli/ Tietze/ Asigner / A3 coupling and other named MCRs, critical analysis of classical MCRs, Relevance of MCR to DOS, Examples from literature

#### **Unit V – Introduction to Bio-conjugation:**

principles and practices: Meaning, Scope and principles of bio-conjugation. Concept of bioorthogonality, common bio-orthogonal functionalities and organic reactions used in bio-conjugation reactions examples from literature.

- 1. Essentials of Chemical Biology Andrew Miller and Julian Tanner
- 2. Multicomponent Reactions Jieping Zhu, Hugues Bienaym
- 3. Bioisosteres in Medicinal Chemistry Volume 54 R. Manhold, H. Kubinyi, G. Folkers
- 4. Diversity Oriented Synthesis-producing chemical tools for dissecting biology–David R.Spring
- 5. Diversity Oriented Synthesis Exploring the intersections between chemistry and biology Derek S Tan

# CHEM 4216 Drug Design and Discovery

Learning To create awareness and emphasize the need for interdisciplinary approach in learning Objectives: To recognize the relevance and application of organic chemistry in the study of biological phenomenon. To equip the students with the principles and strategies of contemporary organic synthesis relevant to chemical biology applications.

**Learning** Learners will be able to recognize and appreciate the role of organic synthesis in drug discovery.

#### **Course Content:**

**Unit I – Drug design, discovery, and development** Past and present.

#### **Unit II – Bioisosterism:**

Introduction – role of bioisosterism in drug development programs, classification of bioisostrism, effects of bioisosterism on biological activity, classical examples.

#### **Unit III – Pharmacokinetics of drug action**

Metabolism of drugs, and the role of metabolism in PK and drug safety – ADME, Toxicity, therapeutic index

#### **Unit IV – The strategies**

Molecular design of new drugs for receptors or enzymes

#### Unit V – Self-study Unit

Latest development in drug discovery of selected diseases (self-study and a submission of a term paper).

- 1. An Introduction to Medicinal Chemistry, G. L. Patrick, 5<sup>th</sup> Edn, Oxford University Press, 2013.
- 2. Fundamentals of Medicinal Chemistry, G. Thomas, John Wiley and Sons Ltd, 2003.

### CHEM 4217 Statistical Thermodynamics

**Learning** This course aims to provide fundamentals of statistical thermodynamics. **Objectives:** 

Learning
On completion of the course, the student should be able to: (a) account for the physical interpretation of partition functions and be able to calculate thermodynamic properties of model systems with using Boltzmann -, Fermi- Dirac and Bose-Einstein statistics. (b) account for the physical interpretation of distribution functions and discuss and show how these can be used in calculations of basic thermodynamic properties. (c) calculate physical characteristics of non-ideal gases and liquids using the most common models for fluids.

### **Course Content:**

### **Unit I – Fundamentals:**

Probability and statistics: Binomial, Poisson, Gaussian Distributions, Bose-Einstein, Fermi-Dirac, Maxwell-Boltzmann statistics, and distribution; Macrostate, microstate, Entropy and equilibrium particle distribution; Thermodynamics Properties - Molecular partition function, internal energy and entropy at dilute limit, thermodynamic properties of ideal gas

### **Unit II – Partition Function and Application:**

Partition function and thermodynamic properties – monoatomic, diatomic, and polyatomic systems; Ideal gas mixtures – non-reacting and reacting ideal gas mixtures, Equilibrium constant; Spectroscopy – Temperature, radiative transitions, Einstein coefficients, absorption and emission spectroscopy.

#### **Unit III – Beyond Dilute Limit:**

Crystalline solid, Einstein and Debye theory of crystalline solid, band theory of metals, Photon gas, Planck's distribution law, black body radiation

#### **Unit IV – Canonical Ensembles:**

Canonical, Grand Canonical, Micro Canonical ensembles, methods, Equilibrium properties and fluctuations; Real gases – partition function of real gases, Virial equation of gases, Rigid sphere, square well, Lennard-Jones Potentials.

- 1. Statistical Thermodynamics: Fundamentals and Applications, Normand M. Laurendeau, Cambridge University Press, 2005.
- 2. Statistical Mechanics, Donald A McQuarrie, Viva Books, 2011.
- 3. Perspectives on Statistical Thermodynamics, Yoshitsugu Oono, Cambridge University Press, 2017.

# CHEM 4218 Analytical Techniques in Chemistry

**Learning** The aims are to provide a sound physical understanding of the principles of analytical chemistry and to show how these principles are applied in chemistry and related disciplines - especially in life sciences and environmental science.

LearningStudents will be able to develop analytical methods and perform chemometricOutcome:analysis to understand the diverse aspects of analytical applications.

### **Course Content:**

### **Unit I – Tools and Data Handling:**

Balances, burettes, volumetric flasks, pipettes, calibration of tools, sampling. Errors and Statistics: significant figures, rounding off, accuracy and precision, errors and error analysis, test for significance – t-test, ANOVA test, chi-squared; Calibration methods: regression and correlation

### **Unit II – Separation Techniques:**

Solvent Extraction: distribution Coefficient, distribution ratio, solvent extraction of metals, multiple batch extraction, counter current distribution. – Chromatographic Techniques: classification, theory of chromatographic separation, distribution coefficient, retention, sorption, efficiency and resolution. Column, ion exchange, paper, TLC and HPTLC: techniques and application. – Gas Chromatography: retention time or volume, capacity ratio, partition coefficient, theoretical plate and number, separation efficiency and resolution.

### **Unit III – Spectroscopic Techniques:**

Electromagnetic radiation, absorption, and emission of radiation Instrumentation: sources, monochromators, detectors. - Flame spectrometry: flame emission, AAS, ICP, instrumentation and application. - Absorption spectrometry: UV-VIS, IR, instrumentation, techniques and applications.

#### Unit IV – Titration, gravimetric and Thermal Techniques:

Acid-base titrations, EDTA titrations, Redox titrations, pH titrations, electrogravimetry, voltammetry - Thermogravimetry: instrumentation and techniques, TGA curves, DTA and DSC, applications. Radiochemical methods: decay reactions, growth of radioactivity, radiation detectors, and tracer techniques.

#### Unit V – Analytical techniques in Biology, Archeology and Environmental Science:

Process involved in various application domains, sample preparations for specific domain application, analyzing results from various techniques toward qualitative and quantitative analysis.

- 1. D. C. Harris, Quantitative Chemical Analysis, 8ed, W. H. Freeman, 2010.
- 2. G. D. Christian and J. E. O'Reily, Instrumental Analysis, 2<sup>nd</sup> Ed., Allyn and Balon, 1986
- 3. Encyclopedia of Analytical Chemistry, R A Meyers (editor) Wiley, 2006.

# CHEM 4219 Organic Synthesis and Approaches

**Learning** This course aims to provide the different principles of retro-synthetic analysis to plan **Objectives:** the synthesis of a given target molecule using different reagents, reactants, and reactions.

**Learning** On successful completion of this course, learners will be able to analyse a given target molecule, identify simple reactants and reactions to make various bonds and write a synthetic protocol to synthesise the given target molecule.

### **Course Content:**

### Unit I – Review of C-C and C-heteroatom bond forming reactions:

Reviewing different methods used in making carbon-carbon (C-C), carbon-nitrogen (C-N), carbon-oxygen (C-O), carbon-sulfur (C-S), carbon-halogen (C-X), etc. bonds using different reagents, reactants, and reactions.

### **Unit II – Retrosynthetic analysis:**

Retrosynthetic analysis, disconnection approach, Synthesis of target molecules based on synthon approach.

### **Unit III– Strategies in Synthesis**

Concept of Umpolung – Functional Group Interconversions. Use of directing groups. Protection and deprotection of common functional groups.

### **Unit IV– Total Synthesis**

Synthesis of target molecules through linear and convergent synthesis (Selected examples)

#### Unit V- Problem solving exercise based on synthetic approaches

Practicing the synthesis of complex organic molecules using different strategies (Selected examples)

- 1. Organic Synthesis: The Science Behind the Art, W. A. Smit, A. F. Bochkov and R. Caple, The Royal Society of Chemistry, 1998.
- 2. Modern Organic Synthesis An Introduction, George s. Zweifel and Michael H. Nantz, W. H. Freeman and Company, NY, 2007.
- 3. Organic Synthesis, Disconnection Approach, S. Warren, John Wiley, 1985.
- 4. Organic synthesis: strategy and control, P. Wyatt and S. Warren, John Wiley and Sons Inc., USA, 2007.
- 5. Greene's Protective Groups in Organic Synthesis, T. W. Greene and P. G. M. Wuts, John Wiley and Sons Inc, 4<sup>th</sup> Edn, 2007.

### CHEM 4200 Research Project and Dissertation

- Developing a research question(s).
- Identifying where the research question(s) fits within existing knowledge, often accomplished through a literature review.
- Designing the method of investigating the question and securing the appropriate permissions to conduct your research.
- Collecting and analyzing data/materials, drawing conclusions from that analysis.
- Writing about, presenting, and publishing your findings.

In keeping with NEP 2020 objectives department of Chemistry defines undergraduate research as follows:

Undergraduate research is a scholarly or creative investigation that contributes to the systematic production of new knowledge; it is a meaningful activity undertaken with the guidance of a faculty member or other research mentor(s) and is used to enrich the College academic curriculum and student experience through enhanced critical thinking skills and a greater understanding of a chosen discipline(s) and its methodologies.

Contact program coordinator, faculty advisor about choosing your mentor

### Credit: 12

**23. Syllabus for Minor Courses** 

### Minor 1

# CHEM 1102 Essentials of Chemistry – I

**Learning** This course aims to provide the basic concepts about atoms and molecules, **Objectives:** intermolecular forces, thermodynamics, chemical kinetics, and electrochemistry.

**Learning** After completion of this course, the students will have a basic understanding of various aspects of general chemistry.

### **Course Content:**

### **Unit I – Atoms and Molecules:**

Atomic and molecular masses: molecular formula determination, stoichiometry and chemical change, quantitative analysis; thermochemistry: enthalpy and its consequences; atoms: structure and spectra, introduction to quantum theory; the periodic table: electron configuration and general properties. (Chapters 3, 4, and 5 of Robinson)

### Unit II – Intermolecular Forces, Liquids and Solids; Solutions and Colloids:

Intermolecular forces – properties of liquids and solids: forces between molecules, properties of liquids and solids, structure of crystal and solids. The nature of solutions: the formation of solutions, dissolutions of ionic compounds, dissolution of molecular electrolytes. Macroscopic properties of solutions: solutions of gases in lipids, solutions of liquids in lipids, the effect of temperature on the solubility of solids in water, solid solutions. Expressing concentration: percent composition, molarity, molality, mole fraction. Colligative properties of solutions, colloids chemistry. (Chapters 10, 11, and 12 of Robinson)

### Unit III – Chemical Thermodynamics; Electrochemistry; Oxidation – Reduction:

The first law of thermodynamics, state functions. Work and heat. Galvanic cells and cell potentials: Galvanic cells, cell potentials, standard electrode potentials, circulation of cell potentials, relationship of the cell potential and the equilibrium constant. Batteries: primary cells, secondary cells, fuel cells, corrosion. Electrolytic cells: the electrolysis of molten sodium chloride, the electrolysis of aqueous solutions, electrolytic disposition of metals, Faraday's law of electrolysis. (Chapters 18 and 19 of Robinson)

#### **Unit IV – Chemical Kinetics:**

Rate of reaction and rate laws. The microscopic explanation of reaction rates: introduction to collision theory of reaction rates, activation energy and the Arrhenius equation, elementary reaction, reaction mechanisms, catalysis. (Chapters 13 of Robinson)

# Unit V – Chemical Equilibrium:

An introduction to equilibrium: the state of equilibrium, reaction quotients and equilibrium constants, Le Chatelier's principle, predicting the direction of a reversible reaction, calculation of equilibrium constants. Kinetics and equilibrium: the relationship of reaction rates and equilibrium, reaction mechanisms involving equilibrium. Ionic equilibrium: monoprotic, diprotic, and triprotic acids; properties of Bronsted bases in aqueous solutions, pH, pOH: measurements and significance, solubility products. The Lewis concept of acids and bases. Precipitation and dissolution. (Chapters 14, 15, 16, and 17 of Robinson)

#### **Text Book:**

- 1. General Chemistry, W. R. Robinson, J. D. Odom, H. F. Holtzclaw, Jr., 10<sup>th</sup> Edition, AITBS Publishers, New Delhi.
- 2. General Chemistry, D. D. Ebbing, 7<sup>th</sup> Edition, AITBS Publishers, New Delhi.

#### Minor 2

### Credit: 4

## CHEM 1202 Essentials of Chemistry – II

**Learning** This course aims to provide the basic concepts about structure and bonding, organic reactions, metals, and metal complexes.

**Learning** After completion of this course, the students will have a basic understanding of various aspects of organic and inorganic chemistry.

#### **Course Content:**

### Unit I – Chemical Bonding; Molecular Structures and Models of Covalent Bonds:

Ionic bonding, covalent bonding: oxidation states and Lewis symbol, valence bond theory: Hybridization of atomic orbitals: sp hybridization,  $sp^2$  hybridization,  $sp^3$  hybridization,  $sp^3d$  and  $sp^3d^2$  hybridization, assignment of hybrid orbital to central atoms, hybridization involving double and triple bonds. Molecular orbital theory: Molecular orbitals, molecular orbital energy diagrams, bond order,  $H_2$  and  $He_2$  molecules, diatomic molecules of the second period. (Chapters 6, 7 of Robinson)

### Unit II – Introductory Organic Chemistry: Structure and Bonding at Carbon:

Elemental carbons and compounds. Organic compounds of carbon: alkanes, nomenclature, hydrocarbons. Derivatives of aromatic and non-aromatic hydrocarbons. Polymers: Factors that affect properties of polymers, polymer properties, kinds of polymers. (Chapters 9 and 24 of Robinson)

### **Unit III – Organic Reaction Mechanisms:**

Types of organic reactions – addition, substitution, elimination reactions – interpretation of reaction profiles – introductory treatment. (Chapter 6, 9 and 15 of Solomons)

#### Unit IV – Chemistry of Representative Metals and Semi-Metals:

The elemental representative metals: Periodic relationships among groups, representative metals, chemical compounds. The semi-metals: The chemical behaviour and structures of the semi-metals, occurrence of boron and silicon hydrides, boron and silicon halides, boron and silicon oxides and derivatives. (Chapter 21 and 22 of Robinson)

#### **Unit V – Transition Elements and Coordination Compounds:**

The transition elements, properties of the transition elements, compounds of the transition elements, superconductors. Coordination compounds: Basic concepts, the naming of the complexes, the structures of complexes, isomerism in complexes, uses of complexes. Introduction to bonding: Valence bond theory, properties and bonding. (Chapter 23 of Robinson)

#### **Text Book:**

- 1. General Chemistry, W. R. Robinson, J. D. Odom, H. F. Holtzclaw, Jr., 10<sup>th</sup> Edition, AITBS Publishers, New Delhi.
- 2. General Chemistry, D. D. Ebbing, 7<sup>th</sup> Edition, AITBS Publishers, New Delhi.
- 3. Organic Chemistry, T. W. G. Solomons, 5<sup>th</sup> Edition, John Wiley and Sons, Inc.
#### (Vocational)

## CHEM 2104 Practice of Chemistry – I

**Learning** This course aims to provide hands-on experience in handling chemicals, laboratory **Objectives:** wares, and laboratory equipment.

Learning After completion of this course, the students will be able to handle the chemicals and glassware with proper safety measurements.

## **Course Content:**

The following experiments will be practiced in this semester.

- 1. Preparation of exactly 0.10 N HCl
- 2. Comparison of the melting point of impure and recrystallized benzoic acid
- 3. Qualitative visualization of exothermic and endothermic reactions
- 4. Estimation of antacid tablet
- 5. Estimation of water of crystallization of a hydrated salt

- 1. Vogel's Text Book of Quantitative Chemical Analysis, Mendham et. al., 6<sup>th</sup> Edn., Pearson Education Ltd., Singapore, 2002.
- 2. Vogel's Text Book of Practical Organic Chemistry, Furniss et. al., 5<sup>th</sup> Edn., Pearson Education Ltd., Singapore, 2004.

(Vocational)

# CHEM 2204 Practice of Chemistry – II

**Learning** This course aims to provide hands-on experience in basic measuring methods for various physical and chemical properties.

Learning After completion of this course, the students will be aware of various methods used for the estimation, identification, and preparation of chemical compounds.

## **Course Content:**

The following experiments will be practiced in this semester.

- 1. Estimation of molecular formula of oxide of magnesium
- 2. Density measurement of irregular objects using liquid displacement method
- 3. Preparation of soap from vegetable oils
- 4. Identification of anions by chemical tests
- 5. Identification of cations by chemical tests

- 1. Vogel's Text Book of Quantitative Chemical Analysis, Mendham et. al., 6<sup>th</sup> Edn., Pearson Education Ltd., Singapore, 2002.
- 2. Vogel's Text Book of Practical Organic Chemistry, Furniss et. al., 5<sup>th</sup> Edn., Pearson Education Ltd., Singapore, 2004.

(Vocational)

## Credit: 4

### CHEM 3104 Practice of Chemistry – III

**Learning** This course aims to provide hands-on experience in basic measuring methods for various physical and chemical properties.

Learning After completion of this course, the students will be aware of various methods used for estimation, identification, and preparation.

#### **Course Content:**

The following experiments will be practiced in this semester.

- 1. Identification of simple organic functional groups by chemical tests
- 2. Preparation of a simple polymer
- 3. Paper chromatographic separation of mixture of coloured inks
- 4. Qualitative analysis of hardness of water by micellar effect comparison of soaping effect of various commercial soaps/detergents
- 5. Qualitative identification of non-electrolyte, strong electrolytes, and weak electrolytes by electrical conductance

#### **Text Book:**

 Vogel's Text Book of Quantitative Chemical Analysis, Mendham et. al., 6<sup>th</sup> Edn., Pearson Education Ltd., Singapore, 2002.
Vogel's Text Book of Practical Organic Chemistry, Furniss et. al., 5<sup>th</sup> Edn., Pearson Education Ltd., Singapore, 2004.

# CHEM 3205 Selected Topics in Inorganic Chemistry

**Learning** This course aims to provide the basics of various aspects of inorganic chemistry. **Objectives:** 

Learning On successful completion of this course, the students will be able to correlate transition metal chemistry, coordination chemistry and organometallic chemistry and their importance. Students may appreciate the relevance of inorganic systems in biology.

## **Course Content:**

## **Unit I – Transition Metal Chemistry:**

Early Transition Elements: Introduction and the chemistry of Scandium group, Titanium group, Vanadium group, Chromium group and Manganese group. Late Transition Elements: Introduction and the chemistry of Iron group, Cobalt group, Nickel group, Copper group and Zinc group.

## **Unit II – Coordination Chemistry:**

A brief review of the general characteristics of transition elements, types of ligands, nomenclature of coordination complexes, chelates, chelate effect, geometry and isomerism, Werner, Sidgwick and Valence bond theory.

## **Unit III – Organometallic Chemistry:**

Compounds with transition metal to carbon bonds: classification of ligands, nomenclature, eighteen electron rule; transition metal carbonyls: range of compounds, structure, bonding, vibrational spectra, preparation, reactions.

## **Unit IV – Bioinorganic Chemistry:**

Metal ions in biological systems: heme proteins, hemoglobin, myoglobin, ferritin, transferrin cytochromes; Iron-sulphur proteins: rubredoxin, ferredoxin.

#### Unit V – Solid State Chemistry:

Inorganic Solids: Ionic solids, close packing, radius ratio, ionic radii, lattice energy; crystal structure, cubic systems (SC, BCC, FCC), fluorite, antifluorite, zincblende, rutile; defects in ionic solids; insulators, semiconductors, and superconductivity.

- 1. J. D. Lee, Concise Inorganic Chemistry, 3<sup>rd</sup> ed., ELBS, 1987.
- 2. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2<sup>nd</sup> ed, BH, 1997
- 3. G. L. Miessler Donald and A. Tarr, Inorganic Chemistry, 3<sup>rd</sup> ed, Pearson, 2003
- 4. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books, CA, 1994.
- 5. E. Huheey, Inorganic Chemistry, 4<sup>th</sup> ed., Harper International, 2001.
- 6. A G. Sharpe, Inorganic Chemistry, 3<sup>rd</sup> ed, Addison-Wesley, 1999.
- 7. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3<sup>rd</sup> Edn., John Wiley, 2001.

## Credit: 4

## CHEM 4104: Selected Topics in Organic Chemistry

**Learning** This course aims to provide a basic understanding of organic chemistry, reaction **Objectives:** mechanisms, and applications.

**Learning** Successful completion of this course, the students will become aware of the organic **Outcome:** reactions and importance of organic chemistry in biology.

## **Course Content:**

## Unit I – Substitution, Elimination and Addition Reactions:

 $S_N 1$ ,  $S_N 2$  and  $S_N i$  reactions, factors affecting substitution reactions,  $E_1$  and  $E_2$  elimination reactions, factors affecting elimination reactions, electrophilic addition reactions.

## **Unit II – Oxidation and Reduction Reactions:**

Oxidation of alcohols using metals and metal-free reagents, oxidation of olefins, sulphides, amines, carbonyl compounds, etc. Catalytic and stoichiometric methods of reduction of organic functional groups.

#### **Unit III – Stereochemistry:**

Constitutional isomers and stereoisomers, configurational isomers and conformational isomers of ethane, butane, cyclohexane. R, S configurations, stereochemical outcome of substitution and elimination reactions.

#### **Unit IV – Heterocyclic Chemistry:**

Synthesis and reactions of five- and six-membered heterocyclic molecules-furan, pyrrole, thiophene, pyridine, indole, quinolone, isoquinoline, etc.

#### Unit V – Chemistry of Biomolecules and Drugs:

Structures and function of aminoacids, carbohydrates, nucleic acids, peptides, proteins, etc., and commonly used modern drugs.

- 1. Clayden, Greeves, Warten, Organic Chemistry, Oxford University Press, 2012.
- 2. P.Y. Bruice, Organic Chemistry 7<sup>th</sup> Edition, Pearson Education, India, 2013.
- 3. Thomas L. Gilchrist, Heterocyclic Chemistry 3<sup>rd</sup> Edition, Pearson Education, India, 2005.
- 4. J. A. Joule and K. Mills, Heterocyclic Chemistry at a Glance, Blackwell Publishers, USA, 2007.
- 5. D. L. Nelson and M. M. Cox, Lehninger Principles of Biochemistry 7<sup>th</sup> Edition, W.H. Freeman, USA.

## **CHEM 4105: Selected Topics in Physical Chemistry**

**Learning** This course aims to provide basic of chemistry through thermodynamics, chemical **Objectives:** kinetics electrochemistry and photochemistry.

**Learning** After completion of this course, the students will have a basic understanding of various aspects of physical chemistry.

## **Course Content:**

## Unit I – Thermodynamics:

Laws of Thermodynamics, Thermodynamic functions (U, H, S, G, and A), Maxwell relations-temperature and pressure effects.

## **Unit II – Chemical Kinetics:**

Rates of the chemical reactions, Arrhenius equation, Linear Gibbs energy relations, Hammond postulate, Curtin-Hammett principle - Hammett equation and its Applications-Examples of reaction mechanism.

## **Unit III – Electrochemistry:**

Electrochemical cells, half-cell potentials and cell potentials, determination of activities and activity coefficients of electrolytes- Debye-Huckel Theory-Thermodynamic information from electrochemistry- Nernst equation.

## Unit IV – Phase Transformations and Stability:

Phase rule, thermodynamics of phase transitions, simple mixtures, colligative properties-phase diagrams-two-component systems- azeotropes, eutectics.

#### **Unit V – Photochemistry:**

Electronic excited states, singlet and triplet states, Jablonski diagram, rate of excited state processes, primary quantum yield, quenching, resonance energy transfer (RET).

- 1. P. Atkins, J. de Paula, J. Keeler, Physical Chemistry, 11<sup>th</sup> Edition, Oxford University Press, Oxford, United Kingdom, 2018.
- 2. R. G. Mortimer, Physical Chemistry, 3<sup>rd</sup> Edition, Elsevier Academic Press, United Kingdom, 2008.
- 3. K. J. Laidler, Chemical Kinetics, 3<sup>rd</sup> Edition, Pearson, India. 2003.
- 4. D. A. McQuarrie and J. D. Simon, Physical Chemistry- A Molecular Approach, Viva Books Limited, 1998.

24. Syllabus for Multi-disciplinary Courses

### Multi-disciplinary - 1

## CHEM 1103 Introduction to Chemistry – I

**Learning** This course aims to provide basic chemistry knowledge to the arts/social science major students.

**Learning** After completion of this course, the students will have a basic understanding of various aspects of chemistry.

#### **Course Content:**

### **Unit I – Atomic Structure:**

Subatomic particles in an atom, the nucleus, electrons, Bohr model, quantum mechanical model, electron configurations, energy level diagram, valence electrons, isotopes and ions.

#### **Unit II – Periodic Properties:**

Repeating patterns of periodicity, understanding how elements are arranged in the periodic table, metals, nonmetals, and metalloids, families and periods.

## **Unit III – Chemical Bonding:**

The ionic bond, positive and negative ions, polyatomic ions, ionic compounds, naming ionic compounds. Covalent bond, understanding multiple bonds, naming binary covalent compounds, empirical formula, molecular formula, structural formula, electronegativity, polar covalent bond, water, VSEPR theory.

#### Unit IV – Air:

Earth's atmosphere: divisions and composition, chemistry of the atmosphere, pollution through the ages, automobile emissions, photochemical smog, acid rain, air pollution, water pollution, indoor air pollution, stratospheric ozone: earth's vital shield, carbon dioxide and climate change.

#### Unit V – Water:

Water: some unique properties, water in nature, chemical and biological contamination, groundwater contamination, usage of water, making water fit to drink, wastewater treatment.

#### **Textbook:**

- 1. Chemistry for Dummies, J. T. Moore, Wiley Publishing, Inc., 2003.
- 2. Chemistry for Changing Times, J. W. Hill and T. W. McCreary, 14<sup>th</sup> Edn., Pearson Education Ltd., 2016

## Multi-disciplinary – 2

## CHEM 1203 Introduction to Chemistry – II

**Learning** This course aims to provide the basics of chemistry in day-to-day life to the arts/social **Objectives:** science major students.

**Learning** After completion of this course, the students will have a basic understanding of chemistry involved in day-to-day life.

## **Course Content:**

## Unit I – Chemistry in Everyday Life:

The chemistry of carbon – organic chemistry, hydrocarbons – alkanes, alkenes, alkynes, aromatic compounds. Functional groups – alcohols, carboxylic acids, esters, aldehydes and ketones, ethers, amines and amides.

## **Unit II – Chemistry of Earth:**

Spaceship earth – structure and Composition, silicates and the shapes of things, metals and ores, earth's dwindling resources.

## **Unit III – Polymers:**

Polymerization – making big ones out of little ones, polyethylene, addition polymerization, rubber and other elastomers, condensation polymers, properties of polymers, plastics and the environment.

## Unit IV – Some Serendipitous Discoveries in Chemistry:

Archimedes, vulcanization of rubber, right- and left-handed molecules, William Perkin and a mauve dye, Kekule, discovering radioactivity, Teflon, stick 'em up!! sticky notes, growing hair, sweeter than sugar.

#### Unit V – Nobel Prize in Chemistry:

Sugar and purine synthesis, discovery of the inert gases, radioactive substance, discovery of radium and polonium, Grignard reagent, coordination complex, synthesis of ammonia, synthesis of haemin, carbohydrates and vitamin C, fission of heavy nuclei, alkaloids, transuranium elements.

#### **Textbook:**

- 1. Chemistry for Dummies, J. T. Moore, Wiley Publishing, Inc., 2003.
- Chemistry for Changing Times, J. W. Hill and T. W. McCreary, 14<sup>th</sup> Edn., Pearson Education Ltd., 2016

### Multi-disciplinary – 3

## CHEM 2103 Introduction to Chemistry – III

**Learning** This course aims to provide the basics of chemistry in day-to-day life to the arts/social **Objectives:** science major students.

**Learning** After completion of this course, the students will understand the chemistry involved in day-to-day life.

## **Course Content:**

## Unit I – Foods:

Carbohydrates in the diet, fats and cholesterol, proteins – muscle and much more, minerals, vitamins, and other essentials, starvation, fasting and malnutrition, flavourings – spicy and sweet, food additives – beneficial or dangerous? problems with our food.

## **Unit II – Fitness and Health:**

Calories – quantity and quality, vitamins, minerals, fluids, and electrolytes, weight loss – diets and exercise, measuring fitness – some muscular chemistry, drugs, athletic performance, and the brain.

## Unit III – Drugs:

Scientific drug design: pain relievers – from aspirin to oxycodone, drugs and infectious diseases, chemicals against cancer, hormones – the regulators, drugs for the heart, drugs and the mind, drugs and society.

#### **Unit IV – Household Chemicals:**

Cleaning with soap – synthetic detergents, laundry auxiliaries – softeners and bleaches, all-purpose and special-purpose cleaning products, solvents, paints, and waxes, cosmetics – personal care chemicals.

#### **Unit V – Chemistry Down on the Farm:**

Farming with chemicals – fertilizers, the war against pests – herbicides and defoliants, sustainable agriculture, looking to the future – feeding a growing, hungry world.

### **Textbook:**

- 1. Chemistry for Changing Times, J. W. Hill and T. W. McCreary, 14<sup>th</sup> Edn., Pearson Education Ltd., 2016.
- 2. Chemistry for Dummies, J. T. Moore, Wiley Publishing, Inc., 2003.

**25. Syllabus for Skill Enhancement Courses** 

#### SEC - 1

## Credit: 3

## CHEM 1100 Chemistry Laboratory – I

**Learning** This course aims to provide hands-on experience in handling chemicals, laboratory **Objectives:** wares, and laboratory equipment.

Learning After completion of this course, the students will be able to handle the chemicals and glassware with proper safety measurements.

#### **Course Content:**

The following experiments will be carried out in this semester.

- 1. Preparation of Exactly 0.10 N HCl
- 2. Comparison of melting point of impure and recrystallized benzoic acid
- 3. Qualitative visualization of exothermic and endothermic reactions
- 4. Estimation of anta-acid tablet
- 5. Estimation of water of crystallization of a hydrated salt
- 6. Estimation of molecular formula of oxide of magnesium
- 7. Density measurement of irregular objects using liquid displacement method
- 8. Preparation of soap from vegetable oils

#### **Reference Books:**

- 1. Vogel's Text Book of Quantitative Chemical Analysis, Mendham et. al., 6<sup>th</sup> Edn., Pearson Education Ltd., Singapore, 2002.
- 2. Vogel's Text Book of Practical Organic Chemistry, Furniss et. al., 5<sup>th</sup> Edn., Pearson Education Ltd., Singapore, 2004.

**SEC** – 2

Credit: 3

# CHEM 1200 Chemistry Laboratory – II

**Learning** This course aims to provide hands-on experience in basic measuring methods for various physical and chemical properties.

Learning After completion of this course, the students will be aware of various methods used for the estimation, identification, and preparation of chemical compounds.

## **Course Content:**

The following experiments will be carried out in this semester.

- 1. Identification of anions by chemical tests
- 2. Identification of cations by chemical tests
- 3. Identification of simple organic functional groups by chemical tests
- 4. Preparation of a simple polymer
- 5. Paper chromatographic separation of mixture of coloured inks
- 6. Qualitative analysis of hardness of water by micellar effect comparison of soaping effect of various commercial soaps/detergents
- 7. Qualitative identification of non-electrolyte, strong electrolytes, and weak electrolytes by electrical conductance

#### **Reference Books:**

- 1. Vogel's Text Book of Quantitative Chemical Analysis, Mendham et. al., 6<sup>th</sup> Edn., Pearson Education Ltd., Singapore, 2002.
- 2. Vogel's Text Book of Practical Organic Chemistry, Furniss et. al., 5<sup>th</sup> Edn., Pearson Education Ltd., Singapore, 2004.

#### SEC - 3

## CHEM 2100 Chemistry Laboratory – III

**Learning** This course aims to provide practical experience for the purification, separation, and **Objectives:** quantification of various organic and inorganic compounds.

Learning After completion of this course, the students will be able to do purification, separation, and quantification of various organic and inorganic compounds.

### **Course Content:**

The following experiments will be carried out in this semester.

- 1. Purification of solvent and compounds: crystallization, sublimation, distillation, Soxhlet extraction,
- 2. Separation methods: solvent extraction, paper, TLC, column, ion-exchange chromatography, demonstration of chromatography instrumentation
- 3. Physical Chemistry: density, viscosity, melting point, boiling point, refractive index, conductivity, and others
- 4. Quantitative analysis: Titrimetry, potentiometry, conductometry
- 5. Computational chemistry

## **Reference Books:**

- 1. Vogel's Text Book of Quantitative Chemical Analysis, Mendham et. al., 6<sup>th</sup> Edn., Pearson Education Ltd., Singapore, 2002.
- 2. Vogel's Text Book of Practical Organic Chemistry, Furniss et. al., 5<sup>th</sup> Edn., Pearson Education Ltd., Singapore, 2004.
- 3. D. C. Young, Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems, John Wiley & Sons, 2001.
- 4. D. Rogers, Computational Chemistry using the PC, 3<sup>rd</sup> Edition, John Wiley & Sons, 2001.