Chemistry curriculum

2019

CHEMISTRY UNBOUND: 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 21st century and beyond

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Department of Chemistry, Pondicherry University, since its inception is a leader and trend setter in developing and implementing a relevant model curriculum which has been adapted by several premier institutes in India. Chemistry curriculum 2019, called *Chemistry Unbound*, 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 21st century and the National education policy 2019. 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 the values to survive in the highly competitive knowledge and skilled society.

Vision and Mission

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

Discover, Create and Understand

Design and model molecules that modulate biological processes

Create materials for energy storage, reaction enhancements, and applied materials

Understand the contribution of geometric and electronic structure to function

Inspire and Educate

Inspire a knowledge platform that supports an inventive culture

Educate future leaders about how chemistry underlies living systems and physical processes

Lead and Collaborate

Lead in fostering solutions to problems of global significance by collaborating across many disciplines both within and external to Pondicherry University

To achieve these aims the Chemistry at Pondicherry University must continue to evolve the cutting-edge facilities, world-leading faculty, and top-quality student body that will make transformative science possible.

Vision

Chemists are driving a molecular revolution of unprecedented magnitude and impact, that will transform 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 ever existed. 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 its excellence in the physical, biological and engineering sciences, Chemistry at Pondicherry University is opening new fields and frontiers and fundamentally new and innovative ways to address the increasingly complex scientific, health, energy and environmental problems of our time.

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 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 that empowers students to address and solve challenges of global significance

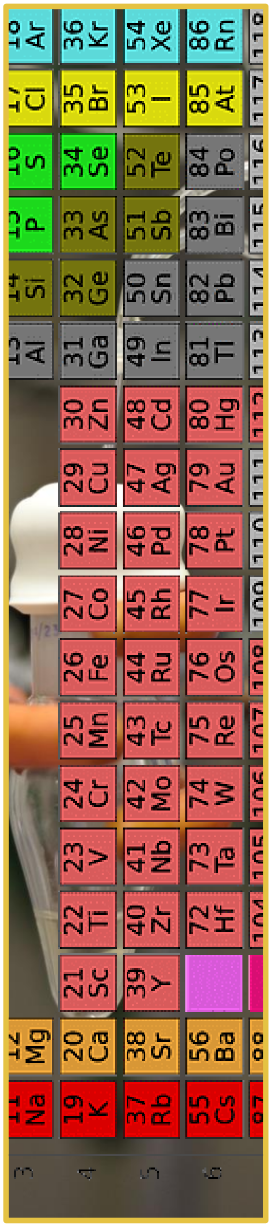
• Reaching out to our future thought leaders—students of all backgrounds from college to doctoral candidates—to share the power of chemistry to create new knowledge directed at the major unmet needs of our time

• 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 by drawing the best faculty and students to the university.



M.Sc. Integrated Chemistry

10 Semester

192 Credits

Inter/Cross disciplinary Options

Research Credits

M.Sc. Five Year Integrated Chemistry

The curriculum of Five years M.Sc. Integrated Chemistry is spread over ten semesters. Considering the key elements of National education policy 2019 with regard to higher education and requirements for obtaining accreditation from professional bodies like American chemical society (ACS) and Royal society of chemistry (RSC), the curriculum is designed to provide an integrated, rigorous educational experience in diverse interdisciplinary and cross disciplinary domains. Course structure consists of basic, foundational and advanced levels in chemistry and from other sciences with an emphasis to begin research from early stages. Curriculum organization is outlined in Chart 1

CHART 1: Overview of M.Sc. Integrated Chemistry Curriculum

M.Sc. Integrated Chemistry
10 Semesters – 192 credits

120 Credits + 72 Credits
Basic + Foundation + Advanced Courses

Exit Option with 120 credits in minimum 6 semesters

Chemistry:
Physics:
Mathematics:
Biology:
Languages:
Environmental science:
Geological Sciences:
Public Administration:

Option for inter-disciplinary and cross-disciplinary choice

Option for undergraduate research

Chemistry:
Physics:
Mathematics:
Biology:
Languages:
Environmental science:
Geological Sciences:
Public Administration:

The program offers a right proportion of a combination of theory and practical based courses. Theory courses are offered at three levels spread over ten semesters. Classroom attendance, interaction with peers, faculty, problem-solving approach and integration with online learning management system are features of the program.

This five-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, project and comprehensive viva are opportunities offered to students to get wide-ranging experiences in research and develop much needed career skills.

Courses offered at first three levels in six semesters are basic in nature, introducing the principles of chemistry. The course content and pedagogy are analytical to facilitate recognition of patterns in chemistry concepts and their connections.

Courses offered at 4^{th} level in two semesters are aimed at laying a strong foundation in professional chemistry education. Organization of course contents and pedagogy are aimed at developing a comprehensive knowledge in chemistry in a unified format going beyond the boundaries of chemistry sub-domains like organic, inorganic etc. and facilitates the students to navigate smoothly towards advanced level courses in any specialized chemistry or related interdisciplinary or cross-discipline domains.

An assortment of courses at an advanced level is offered at 5th level. Students shall have flexibility of choosing courses according to their interest or career planning. These courses are aimed at developing an in-depth knowledge in specialized areas of chemistry and creating an awareness about the relevance and contemporary trends in research.

Practical courses are designed towards equipping the students with skills to enable them to enter into a research career or 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.

Moreover, the proposed curriculum has flexibility to adapt to new programs such as specialization in chemistry, programs of interdisciplinary and cross-disciplinary nature, three-year B.Sc. Chemistry exit option, four-year BS Chemistry program, and also four-year B.Sc.-B.Ed. program.

The rules and regulations of Choice Based Credit System (CBCS) are applicable to this program. Generally, a student takes ten semesters to complete the program. Students may, however, take lesser or greater number of semesters depending on their competence levels and rules and regulations of the University.

A student of five-year M.Sc. Integrated Chemistry program shall acquire a minimum of 192 credits to be eligible to receive the degree certificate. The credit requirements are described in the later pages.

The syllabi given in the following pages are guidelines for the tutors and the students. The course tutor(s) has 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.

Courses offered as specialized topics may adopt alternative methods of evaluation such as submission of term papers, seminar or investigatory project. The course tutor shall clearly define the evaluation methods during the initial meetings of the class and display in her/his web page.

Complete syllabus coverage is a requirement for tutors and students. 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 14 semesters.

Students are advised to go through the credit requirements and course content carefully and plan their curriculum. All students are advised to consult his/her faculty in-charge before choosing the courses in a semester.

Course Evaluation

All courses, generally, are evaluated and awarded grades through two parts (a) continuous assessment (40%) and (b) End semester examination (60%), as prescribed by CBCS regulations of the University. Course tutors may improvise the evaluation procedure in continuous assessment and end semester examination by including, seminar, workshop, discussion, peer-evaluations, review writing, poster presentation etc. in addition to written examinations. However, course tutors shall clearly indicate the evaluation procedure to the students on the first day of the course and provide written instructions in the respective course page online. It is the responsibility of the course tutors appropriately enter the marks and award grades through University SAMS portal.

Course tutors are encouraged to use online technology to assess quality, originality, promptness and enthusiasm of the registered students.

Course Time-Distribution

Credit weightage of the courses are described in accordance with CBCS regulations of the University. This means that a 3-credit course may have approximately 45 lecture hours and a 4-credit course may have approximately 60 lecture hours. This document deliberately does not specify unit-wise time distribution with an intention to allow flexibility to the course tutors. Course tutors are expected to distribute the time among various units of the courses as per the requirement of the course content and students' comprehension.

Overview of the program:

- Credit requirements and Period of Study: 192 Credits / 10 semesters
- Hard-Core Credits: 156 Credits
- Basic courses: 108 Credits
- Foundation Courses: 48 Credits
- Advanced Chemistry Courses: 12 Credits
- Other Courses: 24 Credits
- Laboratory credits aimed at skill development
- Option for undergraduate and graduate research projects
- Flexibility to choose pure chemistry or inter-disciplinary or cross-disciplinary curriculum
- Option for credit transfers from MOOC platform

Program Purpose

The purpose of the five years M.Sc. Integrated Chemistry program at Pondicherry University is to provide the key knowledge base and laboratory resources to prepare students for careers as professionals in the field of chemistry, for graduate study in chemistry, biological chemistry and related fields, and for professional schools including medical, law and business programs, qualified school and college teachers, and more.

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 inter-disciplinary sciences, are eligible to be certified by the American Chemical Society and/or Royal Chemical Society.

- Students will be able to design and carry out scientific experiments as well as accurately record and analyze the results of such experiments.
- Students will develop skills in problem solving, critical thinking and analytical reasoning as applied to scientific problems.
- Students will 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 both 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 and medicine.
- Students will 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.

Credits Distribution

M.Sc. Integrated Chemistry (1-6 semesters): 120 Credits

Chemistry Courses (6*2 Credits*)

Theory Credits (12 courses, HC): 46

Laboratory Credits (6 courses, HC): 16

Physics Department Courses (*13 Credits*)

Theory Credits (2 courses, HC): 6

*Theory Credits (1 course, SC): 3

Laboratory Credits (2 courses, HC): 4

Applied Geology Department Courses (6 Credits)

Theory Credits (2 Courses): 6

Biology and Life Sciences Department Courses (6 Credits)

Theory Credits (2 Courses, HC): 6

Mathematics Department Courses (6 *Credits*)

Theory Credits (2 Courses, HC): 6

Environmental Sciences Department Courses (3 *Credits*)

Theory Credits (3 Courses, HC): 3

Language Department Courses (*12 Credits*)

Functional English (2 Courses, HC): 6

Modern Indian Language (2 Courses, SC): 6

Public Administration Department Courses (*3 Credits*)

Theory Credits (1 Course, HC): 3

Other Schools/Departments/Centres (9 *Credits*)

*Theory Credits (Soft Core): 9

Hard Core Credits (Theory): 88 (73%)

Hard Core Credits (Laboratory): 20 (17%)

Soft Core Credits (Theory) (SC): 12 (10%)

M.Sc. Integrated Chemistry (7 - 10 Semesters): 72 Credits

Foundation Courses

Theory (9 courses, HC): 28

Laboratory (2 Courses, HC): 8

Advanced Chemistry Courses

Laboratory + Project (2 Courses, HC): 8

Seminar + viva + Internship (HC): 4

Theory (4 Courses, SC): 12

Other Courses

*Inter/Cross disciplinary (SC): 12

Core Chemistry Credits (Laboratory + Theory): 60 (83%)

Soft-Core Credits (Theory + Laboratory): 12 (17%)

* Option is available for credit transfers from MOOC platforms

Semester-wise Credit Distribution

A representative semester-wise credit distribution is shown below. Since various schools/departments/centres are involved in offering courses, Chemistry department may reorganize semester credits as per the availability of human resources and infra-structure facilities. Students shall not register for any Soft-Core credits during the first two semesters of their program. Students shall register Soft-Core credits for at least 24 credits from 4th and 5th level courses out of which 12 credits shall be from chemistry courses. The semester-wise credit assignments are only indicative in nature. Students shall register courses as and when they are offered and availability of physical infrastructure. In addition to this, students shall register Functional English, Modern Indian Languages, Environmental Science, Public Administration and other soft-core courses as described in the credit distribution above.

Students are strongly advised to distribute their semester workload equitably and intelligently among semesters for better performance. Students are advised to consult faculty advisor and plan their study.

Courses may have pre-requisites and may also have laboratory and tutorials. Students are encouraged to consult the course tutor before registering. Course tutor shall have the option of waiving the pre-requisites for deserving students.

General Hard-Core (18 Credits)

(These credits are earned as and when they are offered)

Functional English (2 courses, 6 Credits)

Indian Languages (2 courses, 6 Credits)

Environmental Science (1 course, 3 Credits)

Public Administration (1 course, 3 Credits)

Semester 1 (16 Credits)

CHEM110 Introductory Chemistry Laboratory I (2 Credits)

CHEM111 Principles of General Chemistry I (3 credits)

PHYS131 Mechanics (3 Credits)

PHYS130 Physics Laboratory I (2 credits)

MATH116 Calculus - I (3 Credits)

EASC111 Earth and Environment (3 Credits)

Semester 2 (16 Credits)

CHEM120 Introductory Chemistry Laboratory II (2 Credits)

CHEM121 Principles of General Chemistry II (3 Credits)

PHYS140 Physics Laboratory II (2 Credits)

PHYS141 Thermal Physics and Kinetic Theory (3 Credits)

MATH126 Calculus - II (3 Credits)

BIOL101 General Biology I (3 Credits)

Semester 3 (17 Credits)

CHEM210 Chemistry Laboratory 3 (3 Credits)

CHEM211 Inorganic Chemistry (4 Credits)

CHEM212 Mathematics for Chemists (4 Credits)

EASC211 Crystallography and Mineralogy (3 Credits)

BIOL201 General Biology II (3 Credits)

Semester 4 (17 Credits)

CHEM220 Chemistry Laboratory 4 (3 Credits)

CHEM221 Organic Chemistry I: Functionalizing Hydrocarbons (4 Credits)

CHEM222 Introduction to Quantum Chemistry and molecular Symmetry (4 Credits)

PHYS241 Modern Physics (3 Credits)

Soft Core Course (3 Credits)

Semester 5 (18 Credits)

CHEM310 Chemistry Laboratory 5 (3 Credits)

CHEM311: Inorganic Chemistry II (4 Credits)

CHEM312 Organic Chemistry II Functional Group Transformation (4 Credits)

CHEM313 Equilibrium Thermodynamics (4 Credits)

Soft Core Course (3 Credits)

Semester 6 (18 Credits)

CHEM320 Chemistry Laboratory 6 (3 Credits)

CHEM321 Inorganic Chemistry III (4 Credits)

CHEM322 Organic Chemistry III Bioorganic Chemistry (4 Credits)

CHEM323 Chemical Kinetics (4 Credits)

Soft Core Course (3 Credits)

Semester 7 (20 Credits)

CHEM410 Advanced Chemistry Laboratory I (3 Credits)

CHEM411: Symmetry and Structure (3 Credits)

CHEM412: Electronic Structure (3 Credits)

CHEM413: Chemical Bonding (2 Credits)

CHEM414: Chemical Reactions and Energetics (3 Credits)

CHEM415 Chemistry of main group Elements (3 Credits)

*Soft Core Course (3 Credits)

Semester 8 (22 Credits)

CHEM420 Advanced Chemistry Laboratory II (3 Credits)

CHEM421: Reaction Kinetics and mechanism (4 Credits)

CHEM422: Structure and Spectra: Electronic, Vibrational, Microwave (4 Credits)

CHEM423: Structure and Spectra: Magnetic Resonance (4 credits)

CHEM424: Structure and Bonding in Coordination Organometallic Compounds of Transition Metals (4 Credits)

*Soft Core Course (3 Credits)

Semester 9 (15 Credits)

CHEM510 Graduate Research Laboratory (4 Credits)

CHEM511 Summer Internship (2 Credits)

Chemistry Soft-Core Courses (6 Credits)

*Other Soft-Core Courses (3 Credits)

Semester 10 (15 Credits)

CHEM520 Research Project (4 Credits)

CHEM521 Seminar Participation and Review Writing (1 Credit)

CHEM522 Comprehensive Viva (1 Credit)

Chemistry Soft-Core Courses (6 Credits)

*Other Soft-Core Courses (3 Credits)

*Option available to transfer credits from MOOC platform.

Courses List

Laboratory Credits

The above chemistry laboratory courses are intended to impart various experimental and analysis skills to the students. These skills are distributed at various levels and at different semesters. An option to undertake independent undergraduate research project is available for selected students as part of CHEM310 and CHEM320. The following describes details about skills and probable list of experiments.

Probable Skills:

Faculty members may list the experiments on these skill as per their expertise and interests and students choose the relevant skills to work with. Department program committee shall have the right to add, delete and modify skills. A tentative list of experiments is also listed.

- Organizing work space
- Cleaning laboratory apparatus
- Purification of substances
- Weighing, transferring substances
- Stoichiometric estimations
- Property analysis
- Extractions of substances
- Synthesis and characterization
- Ethics and scientific communication

Basic Laboratory Experiments

The following is the list of experiments related to the skills mentioned above. These experiments may be distributed at various levels. Experiments shall be completed in the first six semesters of integrated program. Department Program Committee shall have the right to add, delete and modify experiments.

- To practice prescribed laboratory safety features and handling hazardous chemicals
- Proper handling and calibration of laboratory glassware like pipette, burette, measuring cylinder
- Understanding purity of compounds through melting/boiling point determination
- To prepare standard solutions from molar to ppm by weighing and through dilution
- To perform simple titrations, relevant to chemical, industrial, and agricultural analysis
- To prepare soap and other similar materials
- Measuring density irregular objects and powders through water displacement method
- Measuring viscosity of liquids and solutions
- Estimating stoichiometry
- Simple gravimetric techniques for quantitative analysis
- Qualitative visualization of exothermic and endothermic reactions
- Identification of anions and cations
- Identification of common functional groups
- Preparation of simple polymers, gels, nano particles, colloids,

- Separation technique using paper chromatography
- Soil analysis
- Water analysis
- Spot analysis of inorganic ions
- Functional group analysis
- Thermochemistry experiments
- Equilibrium constant estimation
- Phase equilibrium experiments
- Electrochemistry experiments
- Preparation of buffers
- pH, redox, conductometric titrations
- Conductivity measurements, activity coefficients, equilibrium measurement
- Chromatographic separation
- Simple organic synthesis
- Simple inorganic synthesis
- Simple coordination complex preparations
- Reaction kinetics
- Introducing instrumental analysis
- Using software packages like Excel, Origin, Mathematica, MATLAB to plot, analyze, present

CHEM110 General Chemistry laboratory I

Credits: 2

Given below is the list of experiments as semester wise. These experiments are indicative only and are not restricted only to these. Course tutor may extend, innovate, extrapolate as per the requirements.

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

CHEM120 General Chemistry Laboratory II

Credits: 2

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

CHEM210 Chemistry Laboratory III

Credits: 3

1. Inorganic qualitative analysis: Identifying anions and cations present in the given mixture of inorganic salts. The mixture shall contain an inferring anion.

2. Volumetric analysis involving redox titrations and complexometric titrations.

3. Volumetric analysis involving iodometry

CHEM220 Chemistry Laboratory IV

Credits: 3

1) Identification of well-known organic functional groups - Identification of elements present and functional groups.

2) Determination of phase transition temperature of phenol-water system.

3) Determination of equilibrium constant of $KI + I_2 = KI_3$

4) Phase diagram of two component and three component systems.

5) Electrochemistry experiments.

(i) Determination of electrode potential

(ii) pH titration involving strong/weak acids and strong/weak bases

(iii) Conductometry titration experiments

(iv) Conductivity of weak and strong electrolytes

6) Mini-lab in organic synthesis

(i) Nitration of naphthalene

(ii) Ozazone formation

(iii) Bromination of hydrocarbons

CHEM310 Chemistry Laboratory V

Credits: 3

1. Gravimetric analysis

a) Estimation of barium ions as barium sulphate.

b) Estimation of lead as lead chromate.

c) Estimation of aluminum as its 8-hydroxyquinoline complex

d) Estimation of Ni as Ni DMG complex.

2. Separation of given organic mixture and analysis.

3. Chromatographic techniques TLC, Paper and Column chromatography.

4. Determination of first order rate constant. – Acid hydrolysis of ester

5. Determination of second order rate constant – Base hydrolysis of ester

6. Preparations of gels and colloids

CHEM320 Chemistry Laboratory VI

Credits: 3

1) Separation of cations in a given mixture through ion exchange column and estimation by volumetric / gravimetric methods

2) Extraction of caffeine

3) Isolation of nucleic acid from banana

4) One step synthesis of organic compounds

a) Preparation of chalcone.

b) Bromination of acetaConsult Course Tutoride

c) Epoxidation reaction.

d) Reduction of carbonyl compounds.

e) Preparation of methyl orange.

5) Experiments on analytical chemistry

a) Calibration of burette, pipette and standard measuring flask

b) Estimation of errors from volumetric / gravimetric, and other experiments

c) UV-Vis spectral recording for simple organic inorganic compounds/ions – Theory is not necessary. Experiment should familiarize the techniques to the students

d) IR spectral recording for sample organic/inorganic compounds/ions – To familiarize the technique to the students

e) Solvent extraction of selected organic/inorganic compounds/ions

CHEM111 Principles of General Chemistry I

Credits: 3

Pre-requisite: A pass in higher secondary with mathematics as one of the subjects

Course outcome: On successful completion of this course learners will be able to:

- Comprehend the evolution of electronic structure of atom
- Use quantum numbers and atomic orbital wave function equations to visualize the shapes of orbitals
- Recognize the relationship between position of an element in periodic table and its atomic properties and the periodic trend in properties
- Explain the concept of chemical bonding
- Analyze the properties of gases, liquids, solids and solutions

Course Objectives

1. To develop conceptual knowledge about the electronic structure of atom, organization of periodic table and trend in atomic properties, properties of physical states of matter.

2. Apply the concepts to write electronic configuration of elements. Comprehend, analyze and predict type of chemical bonds and properties of matter.

Course Content:

Unit I Atomic structure

Blackbody emission and temperature, Photoelectric effect, Double slit experiment, Line spectrum of elements, Rutherford's experiment, Bohr's atomic model, Heisenberg's Uncertainty, Quantum atomic model, hydrogen atomic orbitals and quantum numbers, atomic orbital equations (no derivation required), hybrid atomic orbitals, Electronic configuration of atoms, Madelung rule, atomic mass, synthetic elements, isotopes and stability of isotopes (qualitative description)

Unit II Periodic table and periodicity

Periodic trends in atomic properties, reactivity and compound formation, types of compounds, mole concept and composition, oxidation states - Chemical reactions, stoichiometry, chemical reactions in solutions, limiting reagent - Reactions in aqueous medium, precipitation, acid-base, redox, balancing redox reactions, oxidizing and reducing agents, stoichiometry and titration

Unit III Chemical bonding

Types of bonds, representation of electrons as dots, Lewis model of ionic, covalent structures, Electronegativity and bond polarity, Lewis structure of molecular compounds, resonance and 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 IV Gases, Liquids, Solids and Solutions

Gas equations, van der Waals gas, virial gas equation, real gases, intermolecular forces - Properties of liquids, properties of solids, phase diagrams, nature of bonding in solids, crystal structures –

Unit V Solutions

Types of solutions, solution concentration, solubilities of gases, vapour pressure, osmotic pressure, colligative properties of non-electrolyte solutions, electrolyte solutions, colloidal mixtures

Textbook:

Chemistry A Molecular approach, Nivaldo J Tro, 4ed, Pearson, 2017

Further Reading

Chemistry: The Central Science, Theodore L. Brown, H. Eugene LeMay, Jr., Bruce E. Bursten, Catherine J. Murphy, Patrick M. Woodward, Matthew W. Stoltzfus, 13ed, Pearson, 2015

CHEM121 Principles of General Chemistry II

Credits: 3

Pre-requisite: A pass in higher secondary with mathematics as one of the subjects

On successful completion of this course learners will be able to apply the basic principles of chemistry in comprehending and investigating chemical reactions.

Objectives

1. To develop the concept of equilibrium and its application to study chemical phenomenon.

2. To introduce the concept of radioactivity and its applications.

3. To introduce the basic principles og metallurgy.

4. To introduce organic functional groups and biomolecules.

Course Content:

Unit I Chemical Equilibrium

The Concept of Dynamic Equilibrium, The Equilibrium Constant (K), Heterogeneous Equilibria: Reactions involving Solids and Liquids, Calculating the Equilibrium Constant, The Reaction Quotient: Predicting the Direction of Change, Finding Equilibrium Concentrations, Le Châtelier's Principle, solubility equilibria, complex ion equilibria

Unit II Acids and Bases

Definitions, Acid strength and acid dissociation constant, auto ionization of water and pH, strong and weak acids, base solutions, buffers, acid-base properties of ions, polyprotic acids, Lewis concept

Unit III Ionic equilibrium and electrochemistry

Buffers, range and capacity, titration pH curves - Balancing redox reactions, Galvanic cells and spontaneous chemical reactions, standard electrode potential, cell potential, free energy and equilibrium constant, corrosion

Unit IV Radioactivity and metallurgy

Discovery, types, valley of stability of nucleus, detection, kinetics of radioactivity, fission, mass defect and nuclear energy, fusion, nuclear transmutation and trans-uranium elements, application in medicine – natural distribution of metals, metallurgical processes, metal structure and alloys, basic information about transition metals

Unit V Organic Chemistry and Biochemistry

Nature of carbon, hydrocarbons, hydrocarbon reactions, aromatic hydrocarbons, functional groups: alcohols, aldehydes, ketones, carboxylic acids, esters, ethers, amines – Lipids, carbohydrates, proteins and amino acids, protein structure, nucleic acids, DNA

Textbook:

Chemistry A Molecular approach, Nivaldo J Tro, 4ed, Pearson, 2017

Further Reading

Chemistry: The Central Science, Theodore L. Brown, H. Eugene LeMay, Jr., Bruce E. Bursten, Catherine J. Murphy, Patrick M. Woodward, Matthew W. Stoltzfus, 13ed, Pearson, 2015

CHEM211 Basic Inorganic Chemistry I

Credits: 4

Pre-requisite: A pass in higher secondary

Learning Objective: Understand periodic trends and chemistry of various elements. Students after completing this course may relate chemical properties of various elements with respect to their position in the periodic table.

Course Content:

Unit I (Hydrogen and Hydrides, Alkali and Alkaline earth Metals)

Hydrogen and Hydrides: Electronic structure, abundance, preparation and properties, isotopes, ortho- and 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 and Carbon group – Basic treatment)

Boron group: Introduction, diborane and hydrogen compounds of the other elements, 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 (Carbon group)

Introduction, Intercalation compounds of graphite, hydrides, 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 IV (Halogens and noble gases- Basic treatment)

Introduction; hydrogen halides; general considerations of halides; 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 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.

Textbook:

A. G. Sharpe, Inorganic Chemistry, 3rd Edition, Addison-Wesley, 1999.

Further Reading

J. D. Lee, A New Concise Inorganic Chemistry, 3rd Edition., ELBS, 1987.

D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, ELBS. 1990

CHEM212 Mathematics for Chemists

Credits: 4

Pre-requisite: Working knowledge in Calculus

Course Objective and Outcome:

Principles of mathematics are essential to relate various chemical properties and their structures. This course prepares students to understand essential mathematical principles required to understand quantum chemistry, chemical bonding, group theory, spectroscopy and perform computational chemistry calculations.

Course Content:

Unit I Algebra

Complex numbers, vector algebra, polynomials, solving simultaneous equations

Unit II Calculus

Derivative of specific functions, useful derivative identities, Newton's method, Higher-Order Derivatives, Limiting Values of Functions, maximum minimum functions, L'Hospital rule Integrals: The Process of Integration, Improper Integrals, Techniques of Integration, Numerical Integration - Functions of Several Independent Variables, Changes in a Function of Several Variables, Partial Derivatives, Useful Partial Derivative Identities, Thermodynamic Variables Related to Partial Derivatives, Exact and Inexact Differentials, Maximum and Minimum Values of Functions of Several Variables, Vector Derivative Operators - Line Integrals, Multiple Integrals

Unit III Mathematical Series

Constant Series, Power Series, Fourier series, Other Functional Series with Orthogonal Basis Sets, Integral Transforms

Unit IV Differential Equations

Homogeneous Linear Differential Equations with Constant Coefficients, Inhomogeneous Linear differential Equations: The Forced Harmonic Oscillator, Differential Equations with Separable Variables, Exact Differential Equations, Solution of Inexact Differential Equations Using Integrating Factors, Partial Differential Equations, Solution of Differential Equations Using Laplace Transforms, Numerical Solution

Unit V Matrix algebra

Mathematical Operators, Symmetry Operators, The Operation of Symmetry Operators on Functions, Matrix Algebra, Determinants, An Elementary Introduction to Group Theory, Symmetry Operators and Matrix Representations, Cramer’s Rule, Solution by Matrix inversion, Gauss–Jordan Elimination, Linear Homogeneous Equations, Matrix Eigenvalues and Eigenvectors

Unit 6 Using Mathematics software

Use of Mathematica and MATLAB for above units

Textbook:

Mathematics for Physical Chemistry, Robert G Mortimer, 4ed, Elsevier, 2013

Further Reading

Mathematics for physical chemistry, Donald A McQuarrie, University Science, 2008

CHEM221 Organic Chemistry I: Structure and Functionalizing Hydrocarbons

Credits: 4

Pre-requisite: A pass in higher secondary

Learning on: Unique nature of carbon and its bonding property with other elements.

Course outcome:

- The diversity and complexity of binary compound of carbon with hydrogen.
- The effect of structural features on physical and chemical properties.
- The structure and functionalization of hydrocarbons.

Course Content:

Unit I Introduction to organic chemistry

Structure and bonding – types of bonding and shapes of molecules - hybridization, oxidation number, formal charges, resonance; intermolecular forces, introduction to functional groups. Nomenclature of organic compounds.

Unit II Introductory stereochemistry

Types of isomers – constitutional isomers and stereoisomers; configurational isomers, conformational isomers – ethane, butane, cyclohexane; symmetry elements, chirality - compounds with one and two stereogenic centers, optical activity; configurational nomenclature (R/S), representation of stereoisomers – Fischer projection, sawhorse, Newman projection formulae, achiral diastereomers.

Unit III Functionalization of alkanes

Free radical halogenation and other oxidations. Introduction to C–H activation/ functionalization.

Unit IV Functionalization of alkenes, dienes and alkynes All addition reactions

Unit V Chemistry of aromatic hydrocarbons

Aromaticity, Huckel rule, inductive and mesomeric effect, structure and reactions of benzene, Activity and orientation of substituted benzenes. Introduction to other aromatic systems.

Text book:

Organic Chemistry, P. Y. Bruice, Pearson Education, 7ed, 2013

Further Reading:

1. Organic Chemistry as Second Language, David R Klein, 2004, John Wiley and Sons, USA.

2. Arrow Pushing in Organic Chemistry, Daniel. E. Levy, 2008, John Wiley and Sons, USA

3. Organic Chemistry, W. H. Brown, C. S. Foote, B. L. Iverson and E. V. Anslyn, Brooks/Cole Cengage Learning, 6ed, 2012

CHEM222 Introduction to Quantum Chemistry and molecular Symmetry

Credits: 4

Pre-requisite: CHEM212 or a strong foundation in calculus and solving differential equations.

Course Description:

This course will explore the application of quantum mechanics to understanding chemical phenomena, with special emphasis on atomic structure and properties. The postulates of quantum mechanics will be introduced and applied to simple systems. Examination of the simple, yet practically useful, harmonic oscillator and rigid rotor systems will lead into discussion of hydrogenic atoms and hybridization.

Intended Outcomes for the course:

- Apply the postulates of quantum mechanics to simple systems of chemical interest, such as the particle-in-a-box, harmonic oscillator, rigid rotor, hydrogenic atoms, hybrid orbitals.
- Students shall be able to visualize atomic orbitals of hydrogenic atoms
- Shall have ability to solve introductory problems in quantum mechanics
- Shall have ability to identify various molecular symmetry elements and their operations and construct group multiplication table and character table.

Course Content:

Unit I: Blackbody radiation - photoelectric effect - Hydrogen emission and Rydberg formula - Louis de Broglie postulate - Bohr theory - Heisenberg Uncertainty

Unit II: Classical wave equation - oscillating string - superposition of normal modes - vibrating membrane - Schrodinger equation and particle in a box – - Eigen values - quantized energy values and quantum number - uncertainty principle - probabilistic interpretation of wave function - free particles – particle in rectangular well – tunnelling

Unit III: Postulates and General principles in quantum mechanics - properties of operators, Eigen functions, Eigen values, normalization, orthogonality, commuting and non-commuting operators

Unit IV: Solution to Harmonic Oscillator - solution to rigid rotor - solution to hydrogen atom - quantum numbers - atomic orbitals - Hybrid atomic orbitals - construction and visualization of hybrid atomic orbitals - sp, sp2, sp3, dsp2, dsp3, d2sp3 - shape and directional behaviour

Unit V: Symmetry elements and Operations, point groups, non-degenerate representations

Textbook:

Physical Chemistry, A molecular approach, Donald A McQuarrie and John D Simon, 1998, Viva Books Limited

Unit5: Molecular symmetry and Group Theory, A programd introduction to chemical applications, Alan Vincent, 2ed, John Wiley, 2001

Further Reading

Quantum Chemistry, Ira N Levine, 7ed, Pearson, 2014

Chemical Application of Group Theory, F A Cotton, 3ed, John Wiley, 1990

CHEM311: Basic Inorganic Chemistry II

Credits: 4

Pre-requisite: A pass in higher secondary

Course Outline and Outcome: Course describes the nature of coordination compounds and their structures, electronic properties. Students undergoing this course will have working knowledge on synthetic and analysis of coordination compounds and their involvement in biological systems.

Course Content:

Unit I (Coordination Compounds I) Introduction, physical and chemical properties of transition elements; Introduction to coordination compounds; coordination numbers and geometries in transition metal complexes; nomenclature; isomerism in transition metal complexes – structural, geometrical and optical isomerism.

Unit II (Coordination Compounds II) Double salts and coordination compounds; Werner's work; effective atomic number; bonding in transition metal complexes Valence bond theory, crystal field theory (octahedral and tetrahedral complexes); magnetism.

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 (Inner Transition Elements) Lanthanides: Introduction, occurrence, separation, oxidation states and general chemistry.

Actinides: Introduction, isolation and general chemistry

Text Book:

D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, ELBS. 1990.

Further Reading:

1. A. G. Sharpe, Inorganic Chemistry, 3ed, Addison-Wesley, 1999.

2. J. D. Lee, A New Concise Inorganic Chemistry, 3ed, ELBS, 1987.

3. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3ed, John Wiley, 2001.

CHEM312 Organic Chemistry II Functional Group Transformation

Credits: 4

Pre-requisite: A pass in higher secondary and knowledge about writing, identifying various functional groups and their bonding.

Learning on:

- The structure and functionalization of hydrocarbons.
- Electron transmission in organic molecules.
- Course outcome:
- Identify the nucleophile, electrophile and free radical and their reactivity pattern.
- Identify the oxidation states of carbon bearing functional groups.
- Transforming functional groups.

Course Content:

Unit I Identifying and generating Electrophiles and Nucleophiles:

Identifying electrophilic carbons and assigning oxidation number. Identifying and generating carbon nucleophiles and heteroatom nucleophiles.

Unit II Substitution and elimination reactions at sp3 carbon

Nucleophile and electrophiles, Substitution reactions - SN1, SN2 reaction mechanism, factors influencing SN1, SN2 reactions, activation of poor leaving groups, neighbouring group participation, elimination reactions E1, E2, E1cb reaction mechanisms factors affecting, substitutions vs eliminations.

Unit III Reactions of electrophilic unsaturated carbons 1

Reactions of carbon heteroatom multiple bonds, addition reactions to carbon heteroatom multiple bond, addition elimination reactions of carbon heteroatom multiple bond.

Unit IV Reactions of electrophilic unsaturated carbons 2

Reactions of α-carbon to carbon heteroatom multiple bonds. Reactions of α, β unsaturated carbonyl compounds.

Unit V Introduction to radical reactions

Generation of carbon radicals, electrophilic and nucleophilic radical, types of radical reactions.

Text books:

Organic Chemistry, P. Y. Bruice, Pearson Education, 7ed, 2013

Further Reading:

1. Organic Chemistry as Second Language, David R Klein, 2004, John Wiley and Sons, USA.

2. Arrow Pushing in Organic Chemistry, Daniel. E. Levy, 2008, John Wiley and Sons, USA

3. Organic Chemistry, W. H. Brown, C. S. Foote, B. L. Iverson and E. V. Anslyn, Brooks/Cole Cengage Learning, 6ed, 2012.

CHEM313 Equilibrium Chemical Thermodynamics

Credits: 4

Pre-requisite: A pass in higher secondary and working knowledge in basic calculus

Course Outline and Objective: By its origin, thermodynamics is closely related to the study of heat engines and thermodynamic processes. However, the science of thermodynamics should also be understood as the study of thermodynamic properties of substances. In this course, the point of view according to which thermodynamics is concerned with the study of macroscopic properties obtained from macroscopic laws. Students undergoing this course will be equipped to evaluate various thermochemical properties from different experimental variables. From solving problems, students may realise the connection between thermodynamics with biological systems and natural processes.

Course Content:

Unit I: Behaviour of gases and liquids

Real gases, virial equation of state, gas liquid phases - molecular structure of liquids

Unit II First and second laws

First law of thermodynamics, Internal energy, work and heat, enthalpy, effect of enthalpy with temperature, thermochemistry – state functions and exact differentials – Joule Thomson effect – adiabatic changes – Entropy: definitions, Carnot cycle, Clausius inequality, entropy changes in physical processes, measurement of entropy - Third law: Nernst theorem and third law entropy

Unit III System properties and consequences

Helmholtz and Gibbs energies, spontaneous process, maximum work, Standard Gibbs energies – Maxwell relations, temperature, pressure effects on internal, Helmholtz, Gibbs energies, fugacity

Unit IV Physical transformations

Phase stability and phase diagrams, phase rule, thermodynamics of phase transitions – simple mixtures: Partial molar quantities, thermodynamics of mixing, ideal solutions, ideal dilute solutions, excess functions, colligative properties – Phase diagrams: non reacting and reacting binary systems, azeotropes, eutectics, ternary systems

Unit V Equilibrium systems

Activities – solute activity, mean activity coefficients, Debye-Huckel limiting law and theory, activity coefficient – Gibbs energy minimum and equilibrium: effect of temperature and pressure on Gibbs energy change and equilibrium constant Ionic equilibrium: Half-cell reactions and electrodes, types of cells, liquid junction potential, Nernst equation, thermodynamics of cells, determination of standard potentials, activity coefficients, equilibrium constants

Textbook:

Physical Chemistry Thermodynamics, Structure, and Change, Peter W Atkins, Julio de Paula, 10ed, W H Freeman, 2014

Further Readings:

Physical Chemistry, Robert G Mortimer, 3ed, Elsevier, 2008

Physical Chemistry, Thomas Engel and Philip Reid, 3ed, Pearson, 2013

CHEM321 Basic Inorganic Chemistry III

Credits: 4

Pre-requisite: A pass in higher secondary and knowledge in periodic table and periodicity of elements

Course Outline and Objective: 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. Students after completing will be able to predict various reactions of elements and their synthetic methodology.

Course Content:

Unit I (Boron and Carbon Groups-Basic treatment) Compounds of boron with the electronegative elements, metallaboranes and carboranes. Compounds of carbon with the electronegative elements, diamond, graphite, fullerene, carbides.

Unit II (Nitrogen group- Basic treatment) Nitrogen group: Introduction; hydrides; nitrides, phosphides and arsenides; halides, oxo-halides and complex halides; Oxides, oxo-acids and sulphides of N, P, As, Sb and Bi; Phosphazenes; Aqueous solution chemistry; Organic derivatives. Nonaqueous ammonia.

Unit III (Oxygen group- Basic treatment) Oxygen group: Introduction; Hydrides; Halides, Oxo-halides and complex halides, Oxides, Oxo-acids and their salts; Sulphur-nitrogen compounds; Aqueous solution chemistry of S, Se and Te; Organic derivatives. Nonaqueous SO2.

Unit IV (Acids and Bases) Bronsted acids and bases: Bronsted acidy, periodic trends in Bronsted acidy, polyoxo compound formation; Lewis acids and bases: definitions, strengths, representative Lewis acids, heterogeneous acid-base reactions. HSAP principle and its applications.

Unit V (Solid State Chemistry) Inorganic Solids: Ionic solids, close packing, radius ratio, Structure of ionic crystals, ionic radii, lattice energy; crystal structure, defects structures, insulators, semiconductors and superconductivity.

Text book:

D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, ELBS. 1990.

Further Reading:

1. A. G. Sharpe, Inorganic Chemistry, 3ed, Addison-Wesley, 1999.

2. J. D. Lee, A New Concise Inorganic Chemistry, 3ed, ELBS, 1987.

3. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3ed, John Wiley, 2001.

5. L. Jolly, Modern Inorganic Chemistry, 2ed, McGraw-Hill, 1991.

CHEM322 Organic Chemistry III Bioorganic Chemistry

Credits: 4

Pre-requisite: A pass in higher secondary and knowledge about organic functional groups and their reactivity

Learning on:

- The functional group transformations.
- Aromatic hydrocarbons.

Course outcome:

- Effect of replacing carbon/s by heteroatom/s on properties of aromatic hydrocarbons.
- Application of functional group transformations in synthesis of heteroaromatics.
- Recognizing the structure and chemistry of biomolecules.
- Characterizing the simple organic molecules through spectroscopic techniques.

Course Content:

Unit I Chemistry of Heteroaromatics

Chemistry 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

The structure, functions and chemistry of carbohydrates and lipids.

Unit III Amino acids, peptides and proteins

The structure, functions and chemistry of peptides

Unit IV Nucleosides, nucleotides and nucleic acids

Nucleosides and nucleotides, nucleic acids, helical forms of DNA, DNA replication.

Unit V Structural characterization of organic compounds

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

Text book:

Organic Chemistry, P. Y. Bruice, Pearson Education, 7ed, 2013

Further Reading:

1. Heterocyclic Chemistry at a Glance, J. A. Joule and K. Mills, Blackwell Publishers, 2007, USA.

2. Heterocyclic Chemistry, Thomas L. Gilchrist, Pearson Education, 3ed, 2005, India.

3. Organic Chemistry, W. H. Brown, C. S. Foote, B. L. Iverson and E. V. Anslyn, Brooks/Cole Cengage Learning, 6ed, 2012.

4. Organic Chemistry, Leroy G. Wade, Pearson Education; 8ed, 2016, India

CHEM323 Eco-friendly Chemistry – Principles and Practices

Credits: 3

Pre-requisite: Working knowledge in organic function groups reactivity and pattern

On successful completion of this course learners will be able to recognize and appreciate the need for environmentally benign chemistry practices and the principles and methods of practicing eco-friendly chemistry.

Objectives

1. To create awareness about chemical hazards and safety measures.

2. To describe the need and principles of green chemistry.

3. To describe the methods of practicing eco-friendly chemistry

On successful completion of this course learners will be able to recognize and appreciate the need for environmentally benign chemistry practices and the principles and methods of practicing eco-friendly chemistry.

Objectives

1. To create awareness about chemical hazards and safety measures.

2. To describe the need and principles of green chemistry.

3. To describe the methods of practicing eco-friendly chemistry

Course Content:

Unit I Chemical Hazards in the World and Safety Principles,

Principles and Concepts of Green Chemistry, Sustainable Development and Green Chemistry, Atom Economy, Atom Economic Reactions Atom Un-economic Reactions, reducing Toxicity, Waste: Production, Problems and Prevention, Some problems Caused by Waste, Sources of Waste from the Chemical Industry, The Cost of Waste, Waste Minimization Techniques, On-site Waste Treatment, design for Degradation, Recycling

Unit II History of Emergence of Green Chemistry,

Measuring and Controlling Environmental Performance, The Importance of Measurement, Lactic Acid Production, Safer Gasoline, Introduction to Life Cycle Assessment, Green Process Metrics, Environmental Management Systems, IS0 14001, The European Eco-management and Audit Scheme, Eco-labels, Legislation, Integrated Pollution Prevention and Control

Unit III Green Chemistry Principles and Methodologies I

Catalysis and Green Chemistry, Introduction to Catalysis, Heterogeneous Catalysts, Homogeneous Catalysis, Phase Transfer Catalysis, Biocatalysis, Photocatalysis, Organic Solvents: Environmentally Benign Solutions, Organic Solvents and Volatile Organic Compounds, Solvent-free Systems, Supercritical Fluids, Water as a Reaction Solvent, Ionic Liquids, Fluorous Biphase Solvents, Renewable Resources, Biomass as a Renewable Resource, Energy, Chemicals from Renewable Feedstocks, Alternative Economies

Unit IV Green Chemistry Principles and Methodologies II

Emerging Greener Technologies and Alternative Energy Sources. Design for Energy Efficiency Photochemical Reactions, Chemistry Using Microwaves, Sonochemistry, Electrochemical Synthesis

Unit V Designing Greener Processes Conventional Reactors, Inherently Safer Design, Process Intensification, Industrial Case Studies, A Brighter Shade of Green Greening of Acetic Acid Manufacture, EPDM Rubbers, Vitamin C, Leather Manufacture, Tanning, Fatliquoring, Dyeing to be Green,Some Manufacturing and Products Improvements Dye Application, Poly ethane,Eco-friendly Pesticides Chemical The Future's Green: An Integrated Approach to a Greener Chemical Industry, Society and Sustainability, Barriers and Drivers, The Role of Legislation, Green Chemical Supply Strategies

Textbook:

Green Chemistry - An Introductory Text, Mike Lancaster, RSC Publishers, 2002.

Further Reading:

Introduction to Green Chemistry, Albert S. Matlack, Marcel Dekker, Inc. 2001.

CHEM324 Kinetic Theory of Gases and Chemical Kinetics

Credits: 4

Pre-requisite: Higher secondary mathematics

Course Outline: Covers principles of reaction kinetics. Develops understanding of speed distribution of gases, mean speed, root mean speed, diffusion, effusion, and properties of gases. Discussion on properties of ions and ionic compounds. Comprehensive coverage of order, rate, activation energy, effect of catalysis, reaction in solutions. Reaction at surfaces and photoexcited states are also covered.

Intended Outcomes for the course:

- Upon completion of the course students will be able to:
- Understand properties of gases from first principle and can appreciate the concept of pressure and its relation to speed distribution.
- Explain ionic mobility and its consequences.
- Derive and discuss rates of simple and complex reaction kinetics.
- Derive and discuss about surface kinetics and photo excited states kinetics
- Solve problems using kinetic theory of gases and reaction kinetics.

CHEM324 Kinetic Theory of Gases and Chemical Kinetics

Course Content:

Unit I 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 II Introduction: Macroscopic description of non-equilibrium processes, Transport processes, Transport processes in liquids, Electrical conduction in electrolyte solutions: Ionic Motion - mobility of ions - ionic conductivity - strong and weak electrolytes

Unit III Simple Reactions - order of reactions - rate and rate constant - lifetime - activation energy – experiments in determining rate data, reactions in solutions

Unit IV Complex reactions - reversible, consecutive, pre equilibrium, polymerization, explosion, enzymatic reactions - rate equations

Unit V Surface Kinetics and Excited state Kinetics - reactions on surfaces, models in surface kinetics, catalysts and activation energy - electronic excited states - singlet and triplet states, Jablonskii diagrams, rate of excited state processes

Textbooks:

Kinetics and Mechanisms of Chemical Transformations, J Rajaram and J C Kuriacose, Macmillan India Limited, 2011

Further Reading:

1. Chemical Kinetics, Keith J Laidler, 3ed, Pearson India, 2003

2. Physical Chemistry Thermodynamics, Structure, and Change, Peter W Atkins, Julio de Paula, 10ed, W H Freeman, 2014

3. Physical Chemistry - A molecular approach, Donald A McQuarrie and John D Simon, Viva Books Limited, 1998

CHEM325 Physical Chemistry Biology Perspective

Credits: 3

Prerequisites: Higher secondary with mathematics

Enrolment only for non-chemistry major students. Audit Available

Course Description:

This course seeks to present all the material required for a course in physical chemistry for students of the life sciences, including biology and biochemistry. To that end course provides the foundations and biological applications of thermodynamics, kinetics, quantum theory, and molecular spectroscopy. This course shows students how physical chemistry gives quantitative insight into biology and biochemistry.

Intended Outcomes for the course:

Upon completion of the course students will be able to:

- Use thermodynamic terminology correctly.
- Explain fundamental thermodynamic properties.
- Using thermodynamic relations to understand biochemical systems and reactions.

Course Content

Unit I Fundamentals:

Atoms, ions, and molecules- Bonding, nonbonding, structural functional units, Levels of structures - Bulk matter: States of matter, Physical State, Equations of states – Energy: Varieties of energy and Boltzmann distribution.

Unit II Biochemical thermodynamics:

First law, Second Law, Phase equilibria, Chemical equilibrium, Thermodynamics of ion and electron transport

Unit III Kinetics of Biochemical Processes:

Reaction Rates: Rate laws and rate constants, reaction order and determination of rate law – Reaction mechanism: Approach to equilibrium, elementary reactions, consecutive reactions, diffusion-controlled reactions – Reaction dynamics – Enzyme kinetics, transport across membranes and electron transfer kinetics

Unit IV Biomolecular Structures

Microscopic Systems: Principles of quantum theory, hydrogenic atoms, many electron systems – Chemical Bond: Valence bond theory, molecular orbital theory, computational techniques, self-assembly of macromolecules.

Unit V Biochemical spectroscopy

General spectroscopy, vibrational spectra, ultraviolet and visible spectra, radiative and non-radiative decay – Magnetic resonance: Principles of magnetic resonance, information from NMR and EPR

Textbook:

P. W. Atkins, Julio de Paula, Physical chemistry for life sciences. 2ed, 2011

Additional Resources:

Physical Chemistry, Peter Atkins and Julio De Paula, 9th edition 2010, WH Freeman

Advanced Laboratory

This laboratory is designed to introduce research skills and prepare students for undertaking independent research project later in the program and normally offered as fourth and fifth level courses. Students shall, in consultation with the course coordinator, take a published research problem and work on its variation or repeat the same experiment. Students are expected to read the relevant literature, understand experimental variables and characterization techniques and processes. Students shall work in small groups on these experiments and submit report of their work and other documents.

Laboratories credits through CHEM410 and CHEM420 are aimed at developing laboratory skills to undertake independent research in later semesters. Therefore, the present curriculum offers a bouquet of activities and flexibility to the learners instead of rigid prescribed experiments as laboratory component. All faculty members shall participate in these laboratory courses. Each faculty shall suggest, may be at various levels, two to four experiments based on their research expertise and needs. The experiments are prescribed in a way to develop more than one skill in a given experiment, for example, synthesis, separation, characterization, instruments-based analysis, chemical analysis, computational analysis in the same experiment. Many experiments may require more than one laboratory session and therefore students are advised to plan their work accordingly. Experiments may also be of group activity type. Students are advised to consult course coordinator and/or experiment mentor before starting the experiments. Department shall extend all facilities within its limits to complete the experiments Students shall perform experiments in the common laboratory.

To enable students to acquire multiple skills, all faculty members of the department list out experiments on their domain expertise and/or interests. Students are expected to complete 6 experiments (five wet laboratories + 1 computational laboratory) in two semesters and the respective faculty shall award grades to students.

A course coordinator shall perform registration, monitoring, compilation and other logistics. Number of students at any given time for a particular experiment shall be decided by the faculty in-charge for that experiment and shall not exceed five students at any given time. If more students are interested in the same experiment, they shall complete during prior scheduled periods fixed by the faculty in-charge as per his/her convenience. No experiment shall be repeated, except when an advanced skill is acquired by extending additional workout and/or analysis. Students are advised to take experiments as per his/her interests, ability, prior knowledge, requirements for his/her project work. Faculty may depute his/her research student or post-doctorate candidate or guest faculty to undertake this exercise.

Students shall complete at least three experiments suggested by at least three different faculty members in each semester together totaling to six experiments in CHEM400 and CHEM410.

The following are the tentative list of skills

- Single/Multi-step organic synthesis, purification, characterization
- Single/Multi-step inorganic synthesis, purification, characterization
- Preparation of organometallic compounds and characterization
- Preparation of applied materials and characterization

- Preparation of applied polymers and characterization
- Preparation of nano materials and characterization
- Studies involving Steady State emission and time resolved emission
- Studies involving electrochemical techniques
- Characterization of materials through X-Ray crystallography
- Study of kinetics through magnetic resonance
- Studies involving absorption measurements
- Studies involving thermal measurements
- Studies involving electrical and magnetic measurements
- Studying biomolecule interactions with absorption, emission, chromatography, CD etc.
- Electronic structure calculations
- Computational methods in material characterization
- Computational methods in drug discovery
- Studies involving algorithm development and reaction dynamics

Department program committee shall have the powers to add/delete/substitute experiments and/or skills.

CHEM410 Advanced Chemistry Laboratory I

Credits: 3

Pre-requisite: B.Sc. Chemistry or equivalent or should have completed all hard-core credits up to 4th semester of the five-years integrated program

Each experiment shall have the following details.

1. Name of the experiment
2. Skills to be developed
3. Requirements
4. Approximate duration of the experiment
5. Evaluation procedure
6. Related references

Evaluation: Evaluation of each experiment will be of continuous format and evaluated by the faculty in-charge of the experiment.

CHEM420 Advanced Chemistry Laboratory II

Credits: 3

Pre-requisite: B.Sc. Chemistry or equivalent or should have completed all hard-core credits up to 4th semester of the five-years integrated program

Each experiment shall have the following details.

1. Name of the experiment
2. Skills to be developed
3. Requirements
4. Approximate duration of the experiment
5. Evaluation procedure
6. Related references

Evaluation: Evaluation of each experiment will be of continuous format and evaluated by the faculty in-charge of the experiment.

CHEM411: Symmetry and Structure

Credits: 3

Pre-requisite: B.Sc. Chemistry or equivalent or should have earned all hard-core credits up to 4th semester in the five-years integrated program

Learning Outcome: (a) Will be able to identify and assign shapes and molecular symmetry elements (b) will be able construct character tables and identify their significance (c) Visualize, identify, evaluate, 3D molecular structures and energetics of isomers (d) Understand the structural features of solids

Unit I Symmetry Groups: Group Theory Basics – Symmetry Elements, Operations and relationships – Schoenflies Point Groups - Matrix representation and its Character – Classes of symmetry operations - Orthogonality Theorem (without proof) – Construction and Usage of Character tables – Reducible and Irreducible representations – Direct Products – Projection operators.

Unit II Stereochemistry: The Chemistry of Shapes: Configuration and Conformation –Stereoisomers – Conformations around different σ-bonds - Geometries of cyclic systems –Conformer distribution - axial, planar, helical and pro-chirality – Multiple Chiral Centres - Optical activity – Nomenclature.

Unit III Structural feature of aromatics – Aromaticity characteristic features, annulene, benzenoid, nonbenzenoid, heteroaromatics, charged aromatics, fulvenes , fulvalenes, anti aromatics and homoaromatics.

Unit IV Crystals and Structure: Bravais Lattices – Unit cells types – Reciprocal lattice – Brillouin zone – Miller Indices – Classification of Crystal systems and

Bravais lattices – Crystal Classes and Crystal Systems (point and space Groups) – reciprocal lattice - Aperiodic Crystals - Disordered Crystals – diffraction by crystal planes: Laue analysis, Bragg analysis, Ewald synthesis; Chemical Bonding and Lattice Energy: Chemical Bonding and Structure, Lattice Energy, Lattice Energy of Molecular Compounds, Lattice Energy of Ionic Compounds Ionic compounds – Metal packing

Unit V: Chemistry of Shapes in Solids: Polyhedral Types Vertex, Edge and Face, Linked Polyhedra: Vertex-sharing Octahedra, Edge-sharing Octahedra, Face-sharing Octahedra, Octahedra Sharing Edges and Faces - Linked Trigonal Prisms - Vertex-sharing Tetrahedra - Polymorphism and Phase transition, Zintl phases - Symmetry as the Organizing Principle for Crystal Structures: Crystallographic Group–Subgroup Relations, Laves Phases - Interstitial compounds - The Symmetry Principle in Crystal Chemistry, Structural Relationships by Group–Subgroup Relations,

Textbooks:

Symmetry and Spectroscopy of Molecules, K Veera Reddy, 2ed, New Age Science, 2009

Organic Stereochemistry: Stereochemistry of Organic Compounds, Ernst L. Eliel and Samuel H. Wilen, John Wiley and Sons (Asia) Pvt. Ltd., Sigapore, 2003.

Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg (Part A and B) Kluwer Academic / Plenum Publishers, 2000.

Inorganic Structural Chemistry, Ulrich Muller, 2ed, Wiley, 2006

Further Reading:

Introduction to Solid State Physics, Charles Kittel, 8ed, Wiley, 2004

Introduction to Molecular Symmetry (Oxford Chemistry Primers), J S Ogden, 1ed, Oxford University Press, 2001

CHEM412: Electronic Structure

Credits: 3

Pre-requisite: B.Sc. Chemistry or equivalent or should have earned all hard-core credits up to 4th semester in the five-years integrated program

Learning Outcome: (a) Determine the electronic structure of an atom and understand the theoretical basis for the arrangement of electrons (b) Determine the nature of diatomic systems and recognize the nature of bonds, and orbitals

Unit - I Solving Schrodinger's One Electron Atom: The Schrödinger equation – Atomic units – Transformations Relative coordinates- Schrodinger equation in spherical polar coordinates –Separation of variables –Spherical Harmonics – Legendre Equation and its solutions –Interdependency of l and m– The Radial equation and its simplification – Asymptotic solution for ρ equation– interdependency of l and n – Laguerre and associated Laguerre polynomials.

Unit - II Nature of Hydrogenic Wave-functions: Energies and Degeneracies – Justification for Bohr's Energy and Rydberg's formula - Virial Theorem - Angular Momentum– Expressions for Atomic Orbitals –Radial Plots – Probability and Radial Distribution plots –Average and Most probable Distances –Impact of Nuclear Charge variation– Polar plots – Shapes of Atomic orbitals – Planar, Radial Nodes and Orthogonality.

Unit - III Approximations for many-electron Schrodinger equation: Atomic Hamiltonian - Independent Electron Model - Theory of Perturbation - Non-degenerate Perturbation theory - first and second 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 – Effective nuclear charge.

Unit - IV Atomic Structure of many electron atoms: Quantum Particles Indistinguishablity– Electron Spin and its interpretations – Pauli's Antisymmetry principle –Excited states of Helium - Nature of Exchange – Slater Determinants- Slater Type Orbitals – Aufbau principle – Deconstruction of Periodic table – Electron Angular momentum and Spin-Orbit Coupling–Evaluations for Total Angular momentum –Term Symbols – Hund's Rules and its limitations.

Unit V Electronic Structure of Molecules: Bonn-Oppenheimer Approximation – Electronic structure of H2+ - Ground and Excited states of H2– LCAO-MO Theory - VB Theory – Nature of Exchange - HF-SCF Theory –Definition of Chemical bond – Correlation - Configuration interaction - Electronic structure of Homo and Hetero Diatomics of Second Row – Bonds and Lone pairs vs MOs – Bond order – sp Mixing and Avoided Crossing - MO Configuration –Electronic States and Term Symbols.

Textbook:

Quantum Chemistry, Ira N Levine, 7ed, Pearson, 2013

Further Reading:

Quantum Chemistry, Donald A McQuarrie, 2ed, : University Science Books, 2007

CHEM413: Chemical Bonding

Credits: 2

Pre-requisite: Should have earned all hard-core credits up to 4th semester

Learning Outcome: Predict the nature of bond and its properties through various Electronic structural methods; bonding models and intermolecular interactions

Course Content:

Unit I Localized Octet Bonding involving s and p Elements: Review of Classical Bonding ideas – Molecular geometry – Hybridization theory Isovalent hybridization – Bent's rule - VSEPR Theory – FMO theory –- Fundamentals of FMO interaction – Avoided crossing – Jahn-Teller distortions - FMOs of AHn (n=1-4) systems – FMOs A2Hn and ABHN systems – Electronegativity and its perturbation - Bonding in Small rings .

Unit II Delocalized Bonding: Huckel and its Extensions: The simple Huckel method – Assumptions – Determinant, Energies and Wave functions – Extended Huckel and Overlap - Population Analysis Interaction and Walsh diagrams – Conjugation and Aromaticity – Heteroaromaticity – FMOs of Functional groups – Substitutent effects - Hyperconjugation and Anomeric effect – 3D Conjugation - Inorganic Rings.

Unit III Bonding in Solids

Orbitals in periodic potential - Bloch functions and k-space - 1D-Chains and 2D sheets – Energy Bands – Direction and width – Avoided crossings – Folding of bands – Distortions – Density of States and its Projections – Electronic structure of solids – Fermi Energy – Semiconductors, metals and insulators – Band-gap engineering - Population analysis – surface Bonding.

Textbook:

Unit I and II: Fleming, JP Lowe and KA Peterson,

Unit III: R Hoffmann, Solids and Surfaces: A Chemists view of Bonding in extended structures, 1ed, Wiley,

CHEM414: Chemical Reactions and Energetics

Credits: 3

Pre-requisite: B.Sc. Chemistry or equivalent or should have earned all hard-core credits up to 4th semester in the five-years integrated program

Learning Outcome: Student will learn fundamental chemical thermodynamics and be able to use this in experimental and theoretical work with chemical systems, understand the molecular basis for the bulk thermodynamic properties. Students will acquire knowledge to understand and interpret various physical and biological processes in terms of their thermodynamic stability.

Course Content:

Unit I: Fundamentals of Chemical Thermodynamics: Basic concepts and formal postulates - Thermodynamic Temperature Fundamental Equation Entropy Representation -The chemical potential Euler and Gibbs-Duhem equations Legendre transformations (leading to H, G, A, etc.) Quasistatic processes, reversible work and spontaneity Inequalities associated with the 2nd Law Maxwell Relations

Unit II: Selected Applications of Chemical Thermodynamics: Phase transitions, Trouton's rule and Clausius-Clapeyron equation Experimental measurement of Entropy Chemical reaction thermodynamics (in the gas phase) Self-assembling chemical systems Nano-machines and irreversible processes, reactions involved in biological systems, phase stability of minerals, other systems at high-temperature and high-pressures.

Unit III Introduction to Statistical Thermodynamics: Boltzmann factor Partition functions, q and Q Relationship between Q and thermodynamic functions Boltzmann Entropy and Other ensembles

Unit IV Intermolecular Interactions on Chemical Equilibria: Non-ideal gases - the second virial coefficient, Chemical reactions in non-ideal gases, Liquid perturbation theory - the Van der Waals equation, Generalized van der Waals theory of liquids, Equations of state of pure fluids and mixtures Solvent effects on chemical equilibria Ionic solutions - Dielectric continuum approximation

Textbook:

Physical Chemistry: Thermodynamics, Structure, and Change, P W Atkins, 10ed, W. H. Freeman, 2014

Further Reading:

Physical Chemistry, A Molecular Approach, Donald A McQuarrie, 1ed, Viva Publications, 1997

CHEM415 Chemistry of main group Elements

Credits: 3

Pre-requisite: B.Sc. Chemistry or equivalent or should have earned all hard-core credits up to 4th semester in the five-years integrated program

Learning Outcome: Predict, analyse properties of main group elements and their reaction properties and various structural features of compounds formed by these elements

Course Content:

Unit I (Boron)

Synthesis, properties, bonding and structures of B_2H_6, Wades rule - structural features 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.

Unit II (Silicon)

Silanes, cyclosilanes, siloxanes, cyclic siloxanes, Silicon nitrides, Silyl amines, Silicates-classification, 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, sulphur; phosphazines-synthesis, structure, reactivity, applications; comparison with borazine-sulphur-nitrogen compounds-S4N4, S2N2, (SN)x.

Unit IV (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 V (Miscellaneous Topics)

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.

Textbook:

1. F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 6ed, John Wiley, 2004.

2. J. E. Huheey, Inorganic Chemistry, 4ed, Harper International, 2002.

Further Reading:

1. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2ed, BH, 1997.

2. D. F. Shriver, P. W. Atkins, C. H. Langford, 3ed, Inorganic Chemistry, ELBS. 1999.

3. W. L. Jolly, Modern Inorganic Chemistry, 2ed, McGraw-Hill, 1991.

4. M. F. Purcell, J. C. Kotz, Inorganic Chemistry, Saunder, 2010.

5. A. J. Elias, The Chemistry of the p-Block Elements, University Press, 2018.

CHEM421: Reaction Kinetics and mechanism

Credits: 4

Pre-requisite: B.Sc. Chemistry or equivalent or should have earned all hard-core credits up to 4th semester in the five-years integrated program

Learning Outcome: Knowledge about speed of the reaction and its dependence on various variables gives an insight to understand mechanisms of reactions. This course aims towards that. After completing this course, students may understand and write mechanisms for various chemical reactions.

Course Content:

Unit I: Reaction Kinetics: Review of Rate law, Rate constants and order - Experimental methods - 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. Complex reactions: Reversible, consecutive, parallel and competitive, chain reactions – transition state theory – Reactions in solutions: factors influencing the rate, influence of solvent, ionic strength of solution, Kinetic isotope effect, solvent isotope effect – application with selected examples

Unit II Frontier 'sp' orbitals with Linear Transition state: Nucleophiles, Electrophiles and Radicals –Nature of FMOs–Philosophy of Arrow Pushing - Unimolecular and bimolecular processes - Substitution in Saturated and

Unsaturated systems –β and other Eliminations – Elimination vs substitution – Addition across Homo and Hetero nuclear multiple bonds –Electrophilic (Ar) and nucleophilic (RCOOR) Addition-Eliminations – Ring Closure Rules-Regio, Stereo and conformational preferences.

Unit III Frontier 'sp' orbitals with non-linear (Pericyclic) Transition state: Woodward-Hoffmann rules –Electrocyclic reactions – Con and Dis rotatory process - Cycloadditions - Diels-Alder and its Hetero, Retro and Asymmetric variants –Normal and Inverse e n demand - Sigmatropic reactions – Supraand Antra facial Shifts – NIH shift - Ene, Cheletropic and Dyatropic reactions – Site, Stereo, Regio and Peri selectivity – Concerted vs non-concerted pathways – Solvent effects – Arrow-pushing and its limitations- coarctate reactions.

Unit IV Biological perspective of organic reactions: Methyl group transfers - Digestion of carbohydrate by glycosidase - Protein prenyltransferase - Biochemical nucleophilic substitutions with epoxide electrophiles - Nucleophilic substitution over conjugated pi systems

Textbook:

Unit I: Chemical Kinetics, From Molecular Structure to Chemical Reactivity, Luis Arnaut, Sebastio Formosinho, Hugh Burrows, Elsevier, 1ed, 2007

Unit II, III: Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg (Part A and B) Kluwer Academic / Plenum Publishers, 2000.

Unit IV:
https://chem.libretexts.org/Bookshelves/Organic_Chemistry/Book%3A_Organic_Chemistry_with_a_Biological_Emphasis_(Soderberg)

CHEM422: Structure and Spectra: Electronic, Vibrational, Microwave

Credits: 3

Pre-requisite: B.Sc. Chemistry or equivalent or should have earned all hard-core credits up to 4th semester in the five-years integrated program

Course Content:

*Unit 0: Matrix Algebra: Operations in matrices, diagonalization, solution to simultaneous equations, eigen values and eigen vectors

Unit I Theory of Normal Vibrations: Electromagnetic radiation, interaction of electromagnetic radiation with matter, quantum mechanical approach - transition probabilities: Einstein coefficients - pure vibrational and rotational spectra, selection rules, vibrational and rotational spectra of polyatomic molecules, Projection operators and normal modes, anharmonicity, selection rules - Raman effect: classical and quantum theory of Raman effect, rotational and vib-rotational Raman spectra

Unit II (Electronic spectroscopy): Transition moments, assignment of electronic transitions of N2, H2O and formaldehyde using group theory, fluorescence and phosphorescence, ESCA, PES, AUGER techniques

Unit III: Application to organic molecules: UV Visible Spectroscopy: Basic principles, application of UV Visible spectroscopy to organic structure elucidation, Woodward – Fisher rules, Octant rule, Application of ORD – CD to stereochemical assignments. IR – Spectroscopy – Basic principles, characteristic frequencies of common functional

Unit IV: Application to Inorganic Chemistry: Diatomic, triatomic, other geometry and compounds of the p-block elements – Application to Coordination Chemistry – Application to Organometallics – Application to Bio-Inorganic Chemistry

Unit V: Problem solving

Textbook:

Unit 0: Mathematics for physical chemistry, Robert G, 4ed, Elsevier, 2013 (chapter 13)

Unit I, II: Ira Levine, Herzberg (part III),

Unit III: R. M. Silverstein, Pavia

Unit IV: Kazuo Nakamoto

* Students may be asked to prepare the preliminaries through relevant Swayam portal courses

CHEM423: Structure and Spectra: Magnetic Resonance

Credits: 4

Pre-requisite: B.Sc. Chemistry or equivalent or should have earned all hard-core credits up to 4th semester in the five-years integrated program

Course Outline and Objectives: Course describes the basic theory of magnetic resonance applied to chemical systems. Later in the course, the instrumentation study this property and how to this property is employed to solve chemical structures. Students may be asked to record at least one sample (or teacher may share the experimental data). After completing this course should be able to solve chemical structures by identifying various aspects of the spectrum.

Course Content:

Unit I (Magnetic Resonance I: introduction to theory of NMR): Origin of magnetic moments in matter, electronic and nuclear moments, interaction with magnetic field, Larmor equation - conditions for magnetic resonance absorption, relaxation times, line widths and line shapes, chemical shifts, ring currents, diamagnetic anisotropy, spin-spin splitting, high resolution NMR spectra of simple molecules, first and second order treatment of AB systems - FT techniques

Unit II (Magnetic Resonance II): EPR, NQR and Mossbauer spectroscopic techniques - Electron spin resonance: g value, hyperfine structure, esr of organic free radicals, esr of solids, esr of inorganic ions, esr of simple free radicals in solutions - NQR and Mossbauer spectroscopy.

Unit III (Application of NMR Spectroscopy): Instrumentation and principles, Introduction to NMR techniques – CW and FT NMR techniques. 1H 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 1H NMR spectra – NMR of paramagnetic compounds

Unit IV (Multinuclear NMR (with specific emphasis on 13C NMR)): 13C NMR: Proton coupled; off–resonance decoupled; proton noise decoupled 13C 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 1H IH COSY, 1H I3C COSY – HMBC, NOESY and INADEQUATE spectra.

Unit V (Application of mass spectroscopy to organic structure elucidation): Basic principles, techniques of ion production and 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 VI: Problem solving

Textbook:

For Theory: NMR and Chemistry, J. W. Akitt and B. E. Mann, Taylor and Francis, 4ed, 2000

Practical Applications: Spectrometric identification of organic compounds, Robert M. Silverstein, Francis X. Webster, David J, 8ed, 2015, Wiley

CHEM424: Structure and Bonding in Coordination Organometallic Compounds of Transition Metals

Credits: 4

Pre-requisite: B.Sc. Chemistry or equivalent or should have earned all hard-core credits up to 4th semester in the five-years integrated program

Course Outline and Objective: Transition metal complexes are important class of compounds have wide application in biological systems. This course gives a complete knowledge about coordination compounds and their applications. Students may understand and infer various properties of coordination compounds.

Course Content:

Unit I (Introduction to transition metal complexes)

Brief review of the general characteristics of transition elements, types of ligands, nomenclature of coordination complexes, chelates, chelate effect, geometry and isomerism. ORD, CD, Cotton effect.

Unit II (Electronic structure of transition metal complexes 1)

Crystal field theory, crystal field splitting, spectrochemical series, crystal field stabilization energy, application of crystal field theory: crystal field effects on magnetic, thermodynamic properties, ionic radii of transition metal complexes and site preference in spinel structures.

Unit III (Electronic structure of transition metal complexes 2)

MO theory of complexes (quantitative principles involved in complexes with no pi and pi bonding) evidences of pi bonding, electronic spectra of transition metal complexes, Orgel and Tanabe-Sugano diagrams, Jahn Teller distortion, charge transfer and d-d transitions, nephelauxetic series.

Unit IV (Organometallic Chemistry)

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 V (Bioinorganic Chemistry)

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

Text books:

1. P. Powell, Principles of Organometallic Chemistry, 2ed, ELBS, 1991.

2. J. E. Huheey, Inorganic Chemistry, 4ed, Harper International, 2002.

Further Reading:

1. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3ed, John Wiley, 2001.

2. M. F. Purcell, J. C. Kotz, Inorganic Chemistry, Saunder, 2010.

3. F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 6ed, John Wiley, 2004.

CHEM510 Graduate Research Laboratory

Credits: 4

Pre-requisite: None

This laboratory course credit is a prelude to the independent research project work. Students shall register this credit under a chosen/allotted mentorship with whom he/she will continue for his/her research project work. This credit may be used to initiate necessary literature compilation, preliminary experiments, additional skills required for a specific problem, required computational skills etc.

A course coordinator shall be allotted to compile the results and to provide other logistics.

Evaluation: Evaluation shall be done the course mentor/tutor

Generally, evaluation shall be of continuous mode. Various competencies like experimental skills, collection of relevant literature, work ethics, chemistry concepts related to the research project, article writing skills will be tested.

Course mentor/tutor shall inform the students about the evaluation procedure well in advance

CHEM511 Summer Internship

Credits: 2

Pre-requisite: None

Summer internship is another opportunity offered to the students to acquire experience in research or industry. Students may choose to pursue summer internship in one of the research institutes, CSIR laboratories, Universities or manufacturing industries for a period of minimum thirty days.

Students shall submit a work done report endorsed by the mentor/institute or industry authority along with attendance certificate where actually the work was carried out. The format for the endorsement certificate shall be made available to the students

Students are encouraged to go to other institutes or industry to get exposure to diversified work culture and domain knowledge. In case any student is unable to get internship in other institutes or industries, such students shall pursue his/her internship within the department. In such cases students are required to produce evidence with regard to their effort to get internship in at least in two places and denial from those places. If in some unavoidable situation any candidate is not able to pursue summer internship, students with prior approval from the HOD / Project supervisor may do a reading project on frontier area of research in chemistry / interdisciplinary science discipline and submit a literature review.

The internship reports shall be uploaded to our online learning platform and shall be subjected to originality check through appropriate method and the results of this check shall be submitted to the mentor.

Evaluation:

Grading shall be done by evaluation of the submitted report and/or an oral examination.

Evaluation of the report shall be done by a panel of examiners constituted by the department program committee.

CHEM520 Research Project

Credits: 4

Pre-requisite: CHEM410 and CHEM420

This course offers students to get hands on experience of doing research.

Students shall choose or shall be allotted a mentor to undertake the project work. Students shall do supervised mini investigatory project under the mentor.

Students are also encouraged to pursue project in research laboratories of reputed institutes or industries. The project report shall be submitted through online learning platform. After evaluation, students may print a copy of the report signed by the project mentor.

The project reports shall be subjected to plagiarism check through appropriate platform and the results of this check shall be submitted to the mentor.

Evaluation:

- Evaluation shall be done by the mentor.
- The grading shall be done by evaluating the various competencies like originality and quality of the work, work culture, knowledge acquired, and write-up.
- Mentor shall inform the respective students about the grading methods. The general procedure for evaluation shall be decided by the department program committee.

CHEM521 Seminar Participation and Review Writing

Credits: 2

Pre-requisite: CHEM410 and CHEM420

This one credit course is an opportunity to the students to get an idea about the contemporary research areas in chemistry / other science departments / any discipline during their M.Sc. program. Students shall be informed about this course well in advance, normally in the beginning of their program to facilitate enrolment.

Students shall attend a minimum of five seminars, not more than two in any given semester, during their stay. Seminars attended only after the completion of five semesters shall be considered. At least three shall be from chemistry domain and one shall be from other science departments/centres and one from any discipline. Students shall register in their ninth semester of the program for this credit.

The write up shall be submitted through online learning platform and originality shall be evaluated appropriate method and the results of this check shall be submitted to the mentor.

Students shall submit a report describing along with the attendance certificate from the seminar coordinator or organizer in the following format.

1. Title and nature of the of the event

2. Event Coordinator/Organizer
3. Name of the speaker and affiliation
4. Venue / Date and time
5. Abstract:
6. Knowledge gained / relevance
7. Attendance certificate duly signed by event coordinator/organizer
8. Copy of the notification of the event

Students shall undergo an oral examination before a panel of examiners constituted by the department program committee. The topics for the oral examination may also include topics in their research project work (CHEM520), summer internship (CHEM511). Additionally, the examination panel may also include topics from other courses registered by the student in his/her earlier semesters. The examination panel may ask for the reports of CHEM520, CHEM511.

Evaluation:

Grading shall be done by a group of faculty members constituted by the Department Program Committee. Grading shall be based on the originality and quality of the write-up presented by the student and their performance in the oral examination. Marking scheme and grading procedure shall be decided by the department program committee and shall be informed to the students well in advance.

Students shall be informed about the grading methods well in advance by the department.

CHEM551 Structure and Reaction Mechanisms of Transition Metal Compounds

Credits: 3

Pre-requisite: Consult Course Tutor

Course Outcome: Successful completion of this course will make students to relate reactions of inorganic systems and bio-inorganic systems with reference to their structures and electronic property.

Course Content:

Unit I (Reaction mechanisms in transition metal coordination complexes)

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 II (Structure and Bonding in Organometallic Chemistry)

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 (Reactions Mechanisms in Organometallic Chemistry)

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

Unit IV (Bioinorganic Chemistry)

Metalloenzymes: active sites, carboxy peptidase, carbonic anhydrase, superoxide dismutase, catalase and peroxidase, Vitamin B12; photosynthesis, nitrogen fixation, nitrogenase; Na+/K+ ion pump, ionophores, metallodrugs, metal-nucleic acid interaction, nanoparticle drug delivery.

Unit V (Miscellaneous Topic - Applications of Instrumental methods to Inorganic compounds)

Electroanalytical methods, Conductometry, Potentiometry, Polarography, Cyclic Voltammetry; Thermo-analytical methods, TGA, DTA, DSC; Spectroscopic methods, AAS, ICP, AFS, XRF, PES, XPS.

Text books:

1. P. Powell, Principles of Organometallic Chemistry, 2ed, ELBS, 1991.

2. J. E. Huheey, Inorganic Chemistry, 4ed, Harper International, 2002.

3. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3ed, John Wiley, 2001.

Further Reading:

1. M. F. Purcell, J. C. Kotz, Inorganic Chemistry, Saunder, 2010.

2. F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 6ed, John Wiley, 2004.

3. H. H. Willard, L. L. Merritt, J. Dean, F. A. Settoe, Instrumental Methods of Analysis, 7ed, Wadsworth Publishing Co. Ltd. 1988

CHEM552 Selected Topics in Inorganic Chemistry

Credits: 3

Pre-requisite: Consult Course Tutor

Course Objective and Objective: This course aims to relate solid state structures of inorganic systems and their spectral and magnetic properties. Students after completing this course may understand and the relation between magnetic and spectral properties with their structures and may have knowledge in synthesizing materials with desired properties.

Course Content:

Unit I (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 II (Magnetism and Spectroscopy)

Magnetism: Types of magnetism – dia-, para-, ferro- and antiferro-magnetism, quenching of orbital angular moment, spin orbit coupling-Faraday balance, Guoy balance, SQUID, VSM. Resonance Spectroscopy: Applications of NMR, EPR and NQR spectroscopic techniques to Inorganic Compounds.

Unit III (Spectroscopic Analysis of Inorganic Compounds)

Characterization of inorganic compounds by IR, Raman, Mossbauer, UV-vis, MS, electron spectroscopy and microscopic techniques.

Unit IV (Lanthanides and Actinides)

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

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.

Text books:

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. M. F. Purcell, J. C. Kotz, Inorganic Chemistry, Saunder, 2010.

Further Reading:

4. F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 6ed, John Wiley, 2004.

5. D. F. Shriver, P. W. Atkins, C. H. Langford, 3ed, Inorganic Chemistry, ELBS. 1999.

6. J. E. Huheey, Inorganic Chemistry, 4ed, Harper International, 2002.

7. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2ed, BH, 1997

8. S.K. Mehra, Advanced Nuclear Chemistry, Campus Books Internationals, 2009.

CHEM553 Supra-molecular chemistry

Credits: 3

Pre-requisite: Consult Course Tutor

Course Objective and Outcome: Stabilization of chemical systems with non-conventional interactions and synthesis of materials with desired structures are challenging. This course aims at dealing these aspects. Students after completing this course may be in position 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, Calixarens, 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.

CHEM554 Ligand Field Theory (3 credits)

Credits: 3

Pre-requisites: Consult Course Tutor

Course Objective and Outcome: Understanding the bonding of coordination compounds will enable to develop materials with important properties. This course deals about this aspect and students will understand the nature to bonding of ligands with metal ions. Students, after completing this course, shall understand and interpret 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 Oh/Td 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 s >1/2.

Textbooks:

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.

CHEM555 Bio-Inorganic Chemistry

Credits: 3

Pre-requisite: Consult Course Tutor

Course Objective and outcome: Course explains the role of metal ions in various biological processes and systems. 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) - Biodistribution of metal ions-Selection and insertion of metal ions for protein sites-transport and storage proteins- Bioinorganic side of nucleic acid chemistry-Interactions with Metal Ions-Nuclease and Peptidase Models

Unit II (Principles of coordination chemistry linked to Bio-inorganic Chemistry). 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-substitution reactions.

Unit III (Metalloenzymes and Biomimics)

Metalloenzymes- structure activity relationships- Arsphenamine: The first comprehensive structure-activity relationship-blue copper proteins-oxidases-oxygenases-hydrolases-nitrogenase- heme proteins-selected examples-Non-heme centers- Representative examples -Bioinspired metal complexes and their understanding from recent literature.

Unit IV (Physical Methods in Bioinorganic chemistry)

Applications of spectroscopy for understanding biologically important molecules-Electronic spectra, vibrational spectroscopy, CD and MCD-Magnetic resonance methods-NMR, EPR, Mossbauer Spectroscopy-Magnetic measurements-Reduction potential measurements-Electron microscope analysis-X-ray methods-Practical kinetics in bio-inorganic chemistry.

Unit V (Metallodrugs and applications)

Metallodrugs – Therapeutic Agents -Cis-platin-Biochemical mechanisms of DNA damage-DNA repair-cytotoxicity studies-Essential Trace Elements- Nuclear Properties of Metal Ions - Diagnostic Agents- MRI Contrast Enhancement-insight in to recent literature

Textbook:

S.J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books, CA, 1994.

Further Reading:

1. K. D. Karlin and Z. Tyeklar, Bioinorganic chemistry of Copper, Chapman and Hall, Newyork, 1993.

2. W. P. Jencks, Catalysis in Chemistry and Enzymology, McGraw-Hill book company, 1969.

4. Robert A. Scott , Charles M. Lukehart , Applications of Physical Methods to Inorganic and Bioinorganic Chemistry, Wiley Publishers, 2007.

CHEM556 Inorganic photochemistry

Credits: 3

Pre-requisite: Consult Course Tutor

Course objectives: Course explains the reactions of coordination complexes in their photo-excited states. Students shall gain knowledge about various photo-physical and photo-chemical processes involved in coordination complexes.

Course Content:

Unit I (Basic principles)

Absorption of light –photochemical laws – photostationary 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

CHEM557 Catalysis Concepts and Applications

Credits: 3

Pre-requisite: Consult Course Tutor

Course Objectives: To enable to students to understand the structure and properties and their relations of metal complexes based catalysts. The course also aims to give knowledge on various reaction mechanism involving these types of catalysts. Students after completing this course are equipped with designing metal complexes 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.

Text Books 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.

CHEM558: Advanced Organic Chemistry

Credits: 3

Pre-requisite: CHEM312

Learning Outcome:

On successful completion of the course, learners will be able to analyse an organic reaction by applying the principles of thermodynamics and kinetics and describe and predict the possible mechanism of an organic reaction.

Objectives

1. To equip the learners with an in-depth knowledge on the principles, reactivity patterns and paths of organic reactions.

2. To equip the learners with knowledge about generation, characteristics and reactivity of various reactive intermediates.

3. To develop the competence to explore the relationship between organic reactions performed in laboratory and analogous reaction occurring in biological systems.

Course content:

Unit I Introductory physical organic chemistry: Introductory physical organic chemistry, acids and bases – HSAB principle, equilibrium constant thermodynamic effect, kinetic effects – Thermodynamic and kinetic control of organic reactions. Hammond postulate, Curtin-Hammett principle – Hammett equation – Application to organic reactions.

Unit II Stereochemistry and reactivity: Review of basic principles of stereochemistry, axial chirality, planar chirality, helicity, prochirality, other stereochemical descriptors, Configurational and conformational effects on reactivity – Selectivity principles – chemoselectivity, regioselectivity and stereoselectivity, and stereospecificity. Introduction to asymmetric synthesis.

Unit III Reactive intermediates: Reactive carbon species – structure stability, formation and reactivity of carbanion, cabocation, radicals, carbene and benzynes; Reactive heteroatom intermediates – structure, stability, generation and reactions of heteroatom electrophiles and nucleophiles.

Unit IV Rearrangement reactions in organic synthesis: Classification of rearrangement reactions (anionic, cationic and free radical); examples of different kind of rearrangements.

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.

Textbook:

1. Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg (Part A and B) Kluwer Academic / Plenum Publishers, 2000.

Recommended Reading:

1. Stereochemistry of organic compounds, E. L. Eliel, John Wiley, 2003.

2. Reactive intermediates, C. J. Moody and G. H. Whitham, Oxford Chemistry Primers, 1992. 4. Organic Chemistry, S. Ege, AITBS, 2001.

3. Advanced Organic Chemistry - Reaction Mechanisms, R. Bruckner (Academic Press) 2003.

4. A Guidebook to Mechanism in Organic Chemistry, P. Sykes, 6 th Edn, 2003.

5. Principles of Organic Synthesis, R.O.C. Norman and J. Coxon, CRC Press-(Special Indian Edition) 2017.

6. Carruthers, Modern Methods in Organic Synthesis, Academic Press, 1989.

CHEM559 Asymmetric Synthesis

Credits: 3

Pre-requisite: CHEM425

Course outcome

On successful completion of this course learners will be able to explain the need for synthesising biologically active compounds in optically pure form, the principles and strategies of making enantio enriched compounds.

Objectives

1. To recognize the need and effects of enantiomers of biologically active compounds in biological systems.

2. To describe the fundamental principle of achieving enantioselectivity and various methods to achieve enatioselectivity in synthesis.

3. To use the analytical methods to determine the enantioselectivity of a reaction.

4. To investigate the factors influencing the enatioselectivity of a reaction.

Course content:

Unit I Introduction to asymmetric synthesis and resolution:

Asymmetric synthesis Importance and basic principles - Stereoselective and Stereospecific, – Enanatioselective 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 α–chiral carbonyl compounds; Prediction of stereochemistry- Cram's rule and related modifications. Double stereo differentiation; matched pair and mismatched pair; examples from aldol condenzation and hydroboration reactions. Electrophilic addition to α – chiral olefins - epoxidation, cyclopropanation, hydroboration – oxidation, alkylation of enolates of β-chiral carbonyl compounds.

Unit III Asymmetric synthesis using chiral auxiliary:

Chiral Auxilary 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 organo boranes -Application of chiral organoboranes, reduction (Ipc 2 BCl) 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 cyclo addition reactions. Organocatalysis - Proline mediated aldol reactions and further expansion in the field of organo catalysis. Organo cascade reactions. Asymetric Michael addition to α ,β – unsaturated carbonyl compounds.

Reference

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.

CHEM561 Chemistry of Aromatics

Credits: 3

Pre-requisite: CHEM425

Course outcome

On successful completion of this course learners will be able to describe the structural feature, types of aromatic compounds and unique properties of aromatic compounds, predict the properties of aromatic compounds and various methods of synthesis and funtionalization of aromatic compounds.

Objectives

1. To recognize the structural feature of aromatic compounds.

2. To list the types of aromatic compounds.

3. To describe the electronic nature of aromatic compounds.

4. To predict the reactivity pattern of aromatic compounds and tune the reactivity of aromatic compounds.

5. To suggest suitable method for the synthesis of a given hetero-aromatic compound

Course content:

Unit I Aromaticity

Concept of aromaticity, characteristic of aromatic compounds. Types of aromatic compounds – aromatic and anti-aromatic and homoaromatic aromaticity.

Unit II Chemistry of aromatic hydrocarbons

Activation and orientation of mono and di substituted benzenes. Reactivity of fused benzenoids.

Unit III Aromatic Heterocycles I

Chemistry of heteroaromatics with one and two hetero atoms – structure and reactivity.

Unit IV Heterocyclic chemistry II

Chemistry of heteroaromatics with one and two hetero atoms – Synthesis.

Recommended Books:

1. Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg (Part A and B) Kluwer Academic / Plenum Publishers, 2000.

2. Heterocyclic Chemistry, J. A. Joule and K. Mills, Blackwell Publishers, 2010, USA.

3. Heterocyclic Chemistry, Thomas L. Gilchrist, Pearson Education, 3rd Edition, 2005, India.

CHEM562 Organic Synthesis and Approaches

Credits: 3

Pre-requisite: CHEM425

Course outcome

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.

Objectives

1. To describe the principles of retro-synthetic analysis.

2. To apply the tools and techniques of retro-synthetic analysis to plan synthesis of a given target molecule.

3. To identify reactant, reactions and write synthetic a protocol for the synthesis of a given target molecule.

Course content:

Unit I Review of C-C and C-heteroatom bond forming 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

Recommended Books:

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, 4th Edn, 2007.

CHEM563 Organic synthesis – Methodology (Reagents in Organic Synthesis)

Credits: 3

Pre-requisite: CHEM425

Course outcome

On successful completion of this course learners will be able to analyse a given target molecule, identify simple reactants and reagents to make various bonds to synthesize a given target molecule.

Objectives

1. To describe the structural feature, property and role of various organometallic reagents used in organic synthesis.

2. To select a suitable reagent for a given organic transformation.

3. To explain role of the organometallic reagent in a given transformation and explain the mechanism.

Course Content:

Unit I Palladium in Organic Synthesis: The Basic Chemistry of Organopalladium Compounds- Oxidative Reactions with Pd(II) Compounds- Pd(0)-Catalyzed Reactions of sp2Organic Halides and Pseudohalides- Pd(0)-Catalyzed Reactions of Allylic Compounds via Π-Allylpalladium Complexes- Pd(0)-Catalyzed Reactions of 1,3-Dienes, 1,2-Dienes (Allenes), and

Methylenecyclopropanes- Pd(0)-Catalyzed Reactions of Propargyl Compounds- Pd(0)- and Pd(II)-Catalyzed Reactions of Alkynes and Benzynes- Pd(0)-Catalyzed Reactions of Alkenes- Pd(0)-Catalyzed Miscellaneous Reactions of Carbon Monoxide- Miscellaneous Reactions Catalyzed by Chiral and Achiral Pd(II) Complexes.

Unit II Titanium and Indium in Organic Synthesis: Generation of n2-alkyne $Ti(OiPr)_2$ and its utilization in Organic Synthesis, Preparation of Allyl- and Allenyltitanium reagents and their Synthetic Utility-Intramolecular Nucleophilic Acyl Substitution, Intramolecular Couplings of Alkene and Acetylenes-Titanium mediated synthesis of Preparation of Cyclopropanols and Cyclopropylamines - Transformations of Cyclopropanols with cleavage and retention of the cyclopropane ring-Transformation of Cyclopropyamines- Titanium catalyzed epoxide opening -synthesis and reactivity of alkyltitanium derivatives. Indium in Organic Synthesis: Acylation, Hetero Diels-Alder and Michael Addition reaction-Carbonyl Allylation-In-Mediated Allylation, Enantioselective Allylation-Alkynlation-Cross-Coupling Reactions-Radical cyclization-Reduction of Oxime-Azide-Quinoline and Quinoxaline

Unit III Ruthenium and Rhodium in Organic Synthesis: Ruthenium-Catalyzed C–C Bond Formation- Activation of Inert C–H Bonds- Cyclopropanation - Recent Advances in Olefin Metathesis- Ruthenium Vinylidenes and Allenylidenes in Catalysis- Ruthenium Promoted Radical processes towards Fine Chemistry-Selective Carbonylation with Ruthenium catalysts- Organic Synthesis in Aqueous Media-Oxidations using Ruthenium catalysts- synthesis of heterocyclic compounds.

Rhodium-Catalysis: Asymmetric Hydrogenation- Hydroborations-Asymmetric Addition of Organometallic Reagents to Electron Deficient Olefins-Hydroacylation Reactions-Stereoselective Hydroformylation and Silylformylation Reactions -Rhodium(I)-Catalyzed Isomerization reactions- Alder-ene Reaction - Nucleophilic Ring Cleaving Reactions of Allylic Ethers and Amines - Allylic Substitution Reactions - Various types of Cycloadditions- Rhodium(II)-Stabilized Carbenoids Containing both Donor and Acceptor Substituents - Cyclopentane Construction by Rhodium(II)-Mediated Intramolecular C-H Insertion (Taber) - Oxidative Amination- Rearrangement Processes of Oxonium and Ammonium Ylides Formed by Rhodium(II)-Catalyzed Carbene-Transfer.

Unit IV B, Sn, Si, Mg and Cu compounds in Cross-Coupling Reactions: Organoboron Compounds (Suzuki-Miyayura Coupling)- Organostannanes (Kosugi-Migita-Stille Coupling-Organozinc Compounds (Negishi Coupling)-Organomagnesium Compounds- Organosilicon Compounds (Hiyama Coupling)- Organocopper Compounds (Sonagashira Coupling)-Cross Dehyrogenative Coupling Reactions(CDC)-Other Oxidative Coupling reactions.

References

1. Handbook of Organopalladium Chemistry for Organic Synthesis; Negishi, E., Ed.; Wiley-Interscience: New York, 2002.

2. Tsuji, J. Palladium Reagents and Catalysts: Innovations in Organic Synthesis; Wiley and Sons: New York, 1995.

3. Tsuji, J. Palladium Reagents and Catalysts: New Perspectives for the 21st Century; Wiley and Sons: New York, 2003.

4. Palladium in Organic Synthesis; Tsuji, J., Ed.; Springer: Berlin, 2005.

5. Heck, R. F. Palladium Reagents in Organic Synthesis; Academic Press: New York, 1985.

6. Li, J. J.; Gribble, G. W. Palladium in Heterocyclic Chemistry; Pergamon: New York, 2000.

7. Chemistry of Aluminium, Gallium, Indium and Thallium, Downs, A.J. (Ed.)

8. Titanium and Zirconium in Organic Synthesis 1st Edition, Ilan Marek, Victor Snieckus

9. Organotitanium Reagents in Organic Synthesis, Reetz, Manfred

10. Main Group Metals in Organic Synthesis,. Hisashi Yamamoto , Koichiro Oshima, Shuki Araki and, Tsunehisa Hirashita.

11. Ruthenium Catalysts and Fine Chemistry, Christian Bruneau,Pierre H. Dixneuf.

12. C-H Activation: Jin-Quan Yu, Zhangjie Shi.

13. C-H Bond Activation in Organic Synthesis, Jie Jack Li.

14. Modern Rhodium-Catalyzed Organic Reactions- P. Andrew Evan

CHEM564 Selected named organic reactions

Credits: 3

Pre-requisite: Consult Course Tutor

Course outcome:

Learners on successful completion of this course will be able to identify suitable name reaction for a given organic transformation and recognise the relation in given set of named organic reactions.

Objectives

1. To identify a name reaction on a particular concept / functional group.

2. To recognize the relation between given set of name reactions.

3. To select a suitable name reaction for a given organic transformation.

Course content:

Unit I Substitution type reactions

Chichibabin amination reaction, Smiles rearrangement, Finkelstein reaction, Gabriel synthesis, Heine reaction, Kahne glycosidation, Koenigs-Knorr glycosidation, Krapcho dealkoxycarbonylation, Mitsunobu reaction, Myers asymmetric alkylation, Nicholas reaction, Payne rearrangement, Stork enamine synthesis, Williamson ether synthesis, Bischler-Napieralski isoquinoline Synthesis, Combes Quinoline synthesis, Friedel-Crafts acylation, Friedel-Crafts alkylation, Fries rearrangement, Gattermann and Gattermann-Koch Formylation, Houben-Hoesch reaction, Kolbe-Schmitt reaction, Pictet-Spengler tetrahydroisoquinoline Synthesis, Pomeranz-Fritsch reaction, Reimer-Tiemann reaction, Vilsmeier-Haack formylation, von Pechmann reaction

Unit II Reactions involving carbonyl compounds

Aldol reaction, Barbier coupling reaction, Baylis-Hillman reaction, Benzoin and retro-benzoin Condensation, Corey-Chaykovsky epoxidation, Corey-Fuchs alkyne synthesis, Dakin oxidation, Eschweiler-Clarke methylation, Evans aldol reaction, Grignard reaction, Hantzsch dihydropyridine synthesis, Henry reaction, HWE olefination, HWE olefination-Still modification, Kagan-Molander coupling, Keck asymmetric allylation, Knoevenagel condensation, Mannich reaction, Mukaiyama aldol reaction, Passerini multicomponent reaction, Perkin reaction, Peterson olefination, Pictet-Spengler tetrahydroisoquinoline Synthesis, Prins reaction, Reformatsky reaction, Robinson annulations, Roush asymmetric allylation, Sakurai allylation, Seyferth-Gilbert homologation, Stetter reaction, Stobbe condensation, Strecker reaction, Takai-Utimoto olefination, Tebbe olefination, Wittig reaction, Wittig reaction-Schlosser modification

Unit III Reactions involving carbocycle formation and cycloaromatization

Acyloin condensation, Alkene metathesis, Alkyne metathesis, Danheiser cyclopentene annulations, Danishefsky alpha-diene cycloaddition, Dieckmann condensation, Diels-Alder cycloaddition, Hajos-Parrish reaction, Nazarov cyclization, Pauson-Khand reaction, Robinson annulations, Bergman cycloaromatization, Danheiser benzannulation, Dötz benzannulation

Unit IV Reactions involving ring expansion, ring contraction, homologation and fragmentation.

Buchner method of ring expansion, Ciamician-Dennstedt rearrangement, Demjanov and Tiffeneau-Demjanov Rearrangement, Benzilic acid rearrangement, Favorskii rearrangement Skeletal rearrangement, Quasi-Favorskii rearrangement Arndt-Eistert homologation, Corey-Fuchs alkyne synthesis, Doering-LaFlamme allene synthesis, Seyferth-Gilbert homologation Takai-Utimoto olefination, Tebbe olefination, Hofmann rearrangement, Hunsdiecker reaction, Lieben haloform reaction

Text books

1. László Kürti and Barbara Czakó, Strategic Applications of Named Reactions in Organic Synthesis, Elsevier Inc. 2005

2. Jie Jack Li, Name Reactions, Springer-Verlag Berlin Heidelberg 2003, 2006

3. Bradford P. Mundy, Michael G. Ellerd andamp;Frank G. Favaloro, Jr. name reactions and reagents in organic synthesis,II ed, John Wiley andamp; Sons, Inc. 2005

CHEM565 Natural Products Chemistry

Credits: 3

Pre-requisite: CHEM425

Course outcome

On successful completion of this course learners will be able to recognize and appreciate various classes of natural products, their sources, and application and describe the structural feature and biosynthesis of representative examples of each class of natural product.

Objectives

1. To create awareness about the various classes of natural products.

2. To describe the structural feature of representative examples of each class of natural product.

3. To describe and appreciate the biosynthesis of 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 (Poly-phenolics 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 alkaoids; Structure of β-lactam antibiotics (penicillin)

Unit V (Introduction to Marine Natural Products)

Recommended Books:

1. Natural Product Chemistry, K. Nakanishi, Blackie Publications, 3 Vols.

2. Chemistry of Natural Products, R.H. Thomson, Wiley, New York, 1996.

3. Advanced Organic Chemistry, I.L. Finar, ELBS, New Delhi, 1975.

CHEM566 Organic synthesis for chemical biology – principles and practices

Credits: 3

Pre-requisite: CHEM425

Course outcome

On successful completion of this course learners will be able to recognize and appreciate the relevance of organic chemistry to biology, aware of the trend in contemporary organic synthesis to make organic synthesis more relevant to study biological phenomenon.

Objectives

1. To create awareness and emphasize the need for interdisciplinary approach in learning chemistry.

2. To recognize the relevance and application of organic chemistry in the study of biological phenomenon.

3. To equip the students with the principles and strategies of contemporary organic synthesis relevant to chemical biology applications.

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 bio-orthogonality, common bio-orthogonal functionalities and Organic reactions used in bio-conjugation reactions examples from literature.

References:

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

CHEM567 Polymer Science: Synthesis, Characterization

Credits: 3

Pre-requisite: Consult Course Tutor

Course outcome

On successful completion of this course learners will able to describe how structural complexity can be built from simple molecules, general structural feature of monomers, methods of polymer synthesis, characterization and properties of polymers.

Objectives

1. To describe the type of bond in a polymer and rationally design the monomers for a given polymer.

2. To describe various methods used for synthesising polymers.

3. To use the analytical methods to characterize a polymer.

4. To study the properties of polymers.

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 and cationic polymerizations – Living polymerization, Ring opening 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 (T_g) - Factors influencing T_g – Plasticizers – Dilatometry, Differential scanning calorimetry (DSC), Thermomechanical analysis, Dynamic mechanical analysis (DMA). Thermal stability of polymers - Thermo gravimetric 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.

Recommended 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, Jayadev Sreedhar, Polymer Science, New Age International, 2003.

CHEM568 Drug design and discovery

Credits: 3

Pre-requisite: Consult Course Tutor

Course outcome

On successful completion of the course learners will be able to recognize and appreciate the principles drug discovery process, comprehend the structure and functions of targets, interaction between small molecules and targets and their effects, metabolism and excretion of a drug and approaches to rational drug design.

Objectives

1. To describe the structure and functions of drug targets.

2. To describe the types of interaction between a small molecule and the targets.

3. To equip the learners with the principles and strategies for tuning the structure of small molecule to improve the biological relevance of the molecule.

Course content:

Unit I Drug design, discovery and development - Past and present.

Unit II Drug targets – Structure, functions and interactions - receptors, enzymes, proteins, carbohydrates, nucleic acids and lipids.

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 of molecular design of new drugs for receptors or enzymes

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

Recommended Books:

1. An Introduction to Medicinal Chemistry, Graham L. Patrick, 5th Edn, Oxford University Press, 2013.

2. Fundamentals of Medicinal Chemistry, Gareth Thomas, John Wiley and Sons Ltd, 2003.

CHEM569 Chirotechnology

Credits: 3

Pre-requisite: CHEM425, CHEM559

Course outcome

On successful completion of the learners will be able to apply the principles of asymmetric synthesis to develop industrial processes for making important chiral molecules in optically pure form.

Objectives

1. To equip the learners with the principles and practices of obtaining a chiral compound in optically pure form.

2. To impart skills to develop industrial process for making important chiral compounds in optically pure form.

Course content:

Unit I (Basic terminology of stereochemistry)

Description of stereochemistry (glossary of stereochemical terms with specific examples).

Unit II (chirality and biological activity)

Importance of chirality in biology – effect of chirality on pharmacology – pharmacokinetics and pharmacodynamics, effect of chirality on toxicology. Mechanism of biological activity.

Unit III (Source of pure enantiomers – an industrial perspective)

From racemates, from chiral pool compounds, from prochiral substrates.

Unit IV (Determination of enantiomeric purity)

Analytical methods – Polarimeter, Gas chromatography and NMR techniques); assigning absolute configuration.

Unit V (Industrial process of chiral drug synthesis)

Synthesis of chiral drug molecules in industries – comparing different approaches (few drug molecules); Factors effecting process economics; Organocatalytic synthesis of drug molecules.

References:

1. R. E. Gawley and J. Aube, Asymmetric synthesis, 1996

2. R. A. Aitken and S. N. Kilenyi, Asymmetric synthesis, Springer-Science Business Media, B.V., 1992.

3. L. A. Nguyen, H. He, C. Pham-Huy, Int. J. Biomed. Sci., 2006, 2, 85-100.

4. R. A. Sheldon, Chirotechnology: Designing Economic Chiral Syntheses, J. Chern. Tech. Biotechnol. 1996, 67, 1-14 and references cited therein.

5. R. A. Sheldon, Chirotechnology: Industrial Synthesis of Optically Active Compounds, 2nd Edn, 2015.

6. Chirality in Industry, An. N. Collins, G. N. Sheldrake and J. Crosby, John Wiley and Sons, 1992.

CHEM571 Statistical Thermodynamics

Credits: 3

Prerequisite: Knowledge about probability and equilibrium thermodynamics is desirable

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

Textbook:

Statistical Thermodynamics: Fundamentals and Applications, Normand M. Laurendeau, Cambridge University Press, 2005

Suggested Readings:

Statistical Mechanics, Donald A McQuarrie, Viva Books, 2011

Perspectives on Statistical Thermodynamics, Yoshitsugu Oono , Cambridge University Press, 2017

CHEM572 Electroanalytical Techniques

Credits: 3

Pre-requisite: Knowledge about equilibrium and equilibrium electrochemistry is required

Course Description: Electroanalytical techniques offer a unique access to information on chemical, biochemical, and physical systems through applying potential and/or current to the systems. Both the instrumental basis and the theoretical fundamentals are discussed such that non-specialists can easily apply them. This addresses chemists and biochemists who are interested in using electroanalytical techniques to supplement spectroscopic and perhaps theoretical calculations. It also addresses biologists, environmental and material scientists, physicists, medical scientists, and, most importantly, students in all branches of science, who are confronted with the need to apply 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 Impedence.

Textbook:

A. J. Bard and L. R. Faulkner, Electrochemical Methods, Fundamentals and applications, John Wiley, 1980

Recommended Readings:

1. Bockris and Reddy, Electrochemistry, vol 1 and 2, Plenum, 1973.

2. H. Kissinger, Electroanalytical Techniques, John wiley, 1998

CHEM573: Molecular Reaction Dynamics

Credits: 3

Pre-requisite: Knowledge on reaction kinetics and reaction theories is desirable

Course Objective and Outcome: 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 seeks 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.

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 packages (classical and quantum mechanical treatment) – Case studies

Textbooks:

Molecular Reaction Dynamics and Chemical Reactivity, R.D. Levine, R.B. Bernstein (Oxford, New York).

Further Reading:

Theories of Molecular Reaction Dynamics The Microscopic Foundation of Chemical Kinetics, Niels Engholm Henriksen and Flemming Yssing Hansen, Oxford University Press, 2008

CHEM574 Nanomaterial and Photo-catalysis

Credits: 3

Pre-requisite: None

Course Outline: Nanomaterial-based catalysts are usually heterogeneous catalysts broken up into metal nanoparticles in order to speed up the catalytic process. Metal nanoparticles have a higher surface area so there is increased catalytic activity because more catalytic reactions can occur at the same time. This course aims at developing a basic understanding of properties of nano materials and application of such materials in varieties of fields like electronics, solar energy harvesting etc.

Unit I (Nanomaterials)

Nano-science, Fullerene, types of Nanotubes, Molecular Computers

Unit II (Nano-biometrics)

Lipids, templates, proteins, optical memory and DNA, information and Probes, Photodynamic therapy

Unit III (Photonics and Solar Energy)

Photon trapping, nanoholes and photons, formation imaging, solar absorbers, nanostructural polymers, photonic crystals

Unit IV (Nano-electronics and Quantum electronics)

Semiconductors, Transistors, Nanofabrication of Quantum Computers.

Unit V (Nanomaterial Photo-catalysis)

Nanostructured materials, energy conversion and storage

Recommended books:

1. Nanotechnology Basic Science and Energy Technologies, Mich Wilson, Kamali Kanengara, Geoff smith, Michelle Simmons and Burkherd Raguk, Overseas press (I), N.D. 2005.

CHEM575 Solid State Chemistry

Credits: 3

Pre-requisite: None

Course Outline and Objective:

Unit I (Physical Methods for characterizing solids)

X-ray diffraction: powder and single crystal, Neutron diffraction, Electro microscopy, Atomic force microscopy, X-ray absorption and fluorescence, NMR, Thermal analysis

Unit II (Solid State Chemistry-1)

Imperfections and related phenomena- Defects in Solids: Point defects, line defects and plane defects. Thermal properties- Heat capacities of Solids: Dulong-Petit law, Einstein and Debye theories, thermal conductivity of insulators and thermal expansion coefficient. Electrical conductivity- origin of band gap, Fermy energy, density of states, thermal conductivity of metals, semiconductors and superconductivity.

Unit III (Solid State Chemistry-2)

Magnetic properties: classification of magnetic materials, quantum mechanical theory of paramagnetism, nuclear paramagnetism, ferro- antiferro- and ferrimagnetism. Solid state transformations, solid state reactions, theory and techniques of crystal growth.

Unit IV (Solid State Chemistry-3)

Diffusion in solids: diffusion mechanisms, Fick's laws of diffusion, diffusion as a random walk problem. Optical properties: thermionic emission, photovoltaic effect, optical absorption of semiconductors. Dielectric properties: dielectric constant and related properties, behaviour of dielectric materials in ac fields, Clausius-Mosotti equation. Thermoelectric effects: Thompson effects, Peltier effect, Seebeck effect, thermocouples and Hall effect. Hopping semiconductors, polarons, liquid crystals, and glasses. Pauling's rules in polyhedral structural chemistry

Unit V: Surface Chemistry: Introduction to the properties of surfaces, Interactions of atoms and molecules with surfaces, Thermodynamics of surfaces, Introduction to heterogeneous catalysis

Textbook:

Solid State Chemistry – An Introduction, Lesley E Smart, Elaine A Moore, CRC Press, 2012

Further Reading:

1.H. V. Keer, Principles of Solid State, Wiley Eastern Limited, 1993

2. Introduction to Surface Chemistry and Catalysis, 2nd edition, 2010

CHEM576 Analytical Techniques in Chemistry

Credits: 3

Pre-requisite: None

Audit Available

Course Outline and Objective: 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. Students will be trained to develop analytical methods and perform chemometric analysis

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, 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 (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.

Textbook:

D. C. Harris, Quantitative Chemical Analysis, 8ed, W. H. Freeman, 2010

Further Reading:

G. D.Christian and J. E. O'Reily, Instrumental Analysis, 2nd Ed., Allyn and Balon, 1986

Encyclopedia of Analytical Chemistry, R A Meyers (editor) Wiley, 2006

CHEM577 Chromatographic Separation Methods

Credits: 3

Pre-requisite: None

Audit Available

Course Outline and Objective: Chromatographic separations involve a large number of interacting variables that must be optimized in order to achieve the maximum resolution and the minimum analysis time for any given separation. To select the best conditions, it is necessary to understand chromatography theory. Students will be trained to analyze and operate various chromatographic techniques.

Unit I (Fundamentals of Chromatography)

Theory – Retention factor, resolution and theoretical plates, Band broadening, resolution equation, peak symmetry, operating variables, instrumentation, quantification and standardization

Unit II (Gas Chromatography)

Theory – GC Columns and partitioning, operating variables; instrumentation – nature of stationary phase, carrier gas, columns, detectors; Practice – qualitative and quantitative applications, Tandem GC

Unit III (Liquid Chromatography)

Scope, normal and reverse phases, ion-exchange, size exclusion, affinity; HPLC Instrumentation, 2D-LC, qualitative and quantitative applications

Unit IV (Hyphenated Techniques)

GC-MS instrumentation, method development, setup and operation, Ion-trap; LC-MS – Electrospray, ion spray, comparison with GC-MS, selected applications

Textbook:

Chromatography Principles and Applications, Mark F Vitha, Wiley, 2017

Further Reading:

GC/MS A Practical User's Guide, Marvin C McMaster, 2ed, Wiley Interscience, 2008

Chromatography Theory, Jack Cases and Raymond P W Scott, Marcel Dekker, 2002

CHEM578 Computational Quantum Chemistry: Molecules

Credits: 3

Pre-requisite: Knowledge in introductory quantum mechanics and chemical structures.

Course Outline and Objective: This course is primarily intended as a guide to help navigate among different computational methods currently in use. In order to accomplish this goal, it provides a compact description of the basis of computational chemistry along with many examples of applications of these methods in various areas. It is assumed that the students enrolling this course are interested in applications of computational methods, a broad range of the most important applications of computational chemistry is provided. The applications include descriptions of standard chemical calculations for model molecules under various conditions. This course provides information on prediction of various molecular properties as well as investigations of chemical reactions.

Course Content:

Unit I (Hartree-Fock Theory): Molecular Hamiltonian – Bonn-Oppenheimer Approximation – Mean Field Theory – Fock Operator - Trial Wave functions – LCAO approximation - Roothan's equations – Fock matrix – Self-Consistent Field theory – MO andamp; Total Energies – Koopman's Theorem - Open Shell systems – UHF vs ROHF - Broken Symmetry solutions - Spin polarization – Spin contamination.

Unit II (Basis Sets) Single center (vs) Multi center expansions - Slater type Orbitals – minimal vs extended basis sets – split-valence basis sets – Gaussian Type Orbitals – Primitive and Contracted Gaussians – Polarization functions – Diffuse functions – Effective Core Potential (ECP) – Pople's Notation – Basis set Limit - Basis set superposition Error (BSSE) – Counterpoise Correction.

Unit III (Post-Hartree Fock Methods) Static vs dynamic correlation - Configuration Interaction (CI) – CI matrix – Brilloin's Theorem - Slater-Condan rules – Configuration State Functions - Multiconfiguration SCF – Choice of active spaces - Many body perturbation theory – Moller-Plesset (MPn) method - Coupled Cluster Methods – Size Consistency and Extensivity – Time, space complexities.

Unit IV (Density Functional Theory) Electron Density vs Wave functions - Hole functions – Thomas-Fermi model – Slater's Approximation – Hohenberg-Kohn theorems - Kohn-Sham Theory – Exchange and Correlation holes – Local Density Approximation (LDA), Gradient-corrected Methods – Kohn-Sham Orbitals – Hybrid Functionals – Performance of DFT models.

Unit V (Molecular Properties) Geometry optimization – Symmetry - Hellmann-Feynman Theorem - Properties (time dependent and independent) - Normal modes - Vibrational Analysis and characterization of Stationary Points IR /Raman spectra – Anharmonic corrections – Electrical, Magnetic and Thermodynamic properties – Characterizing Transition states - Solvent Models.

References:

1. J. P. Lowe and K. A. Peterson, Elsevier Academic Press, New York, 2006.

2. P. W Atkins and R. S. Friedman: Molecular Quantum Mechanics, Oxford, 2005.

3. F. Jensen, Introduction to computational chemistry, Wiley, NY, 2007.

4. C. J. Cramer, Essentials of Computational Chemistry, John-Wiley andamp; Sons, 2004.

5. A. Szabo and N. S. Ostlund, Modern Quantum Chemistry, Dover, NY, 1996.

CHEM579 Computational Quantum Chemistry: Materials

Credits: 3

Pre-requisite: CHEM578

Course Outline and Objective: This course provides information on prediction of various molecular properties of periodic materials like crystals, amorphous solids, surface properties, catalytic reactions.

Course Content:

Unit I Basics of Quantum Chemical Calculations on Periodic Structures

Schrodinger's Equation – Periodic Potentials - Bloch Functions – Reciprocal Space and kQuantum number – Brillouin Zone - Band Structures

Unit II Advanced Computations

Basis sets – All-electron basis, Atomic-basis, Plane-wave basis – Psuedopotentials – Normconserving, ultrasoft, PAW - Exchange and Correlation - Density Functional Theory - Approximations – LDA and GGA

Unit III Chemical Bonding Descriptors

Density of States – Electron Partitioning Schemes – Population Analysis – Overlap Populations – Extensions of molecular partitioning schemes to periodic systems – periodic EDA – Chemical Pressure indicator - Applications

Unit IV Properties of Materials

Lattice optimizations – Lattice Vibrations – Phonon Calculations – Electronic Excitations - Relativistic Effects – Polarizabilities and Hyper-polarizabilities – Magnetic Resonance – Super-cell calculations

Reading Material

1. Computational Chemistry of Solid State Materials, Ed. Richard Dronskowski, Wiley, 2005

2. Methods of Electronic Structure Calculations, Ed. Michael Springborg, Wiley, 2000

3. Electronic Structure Calculations for solids and Molecules – Jorge Kohanoff, Cambridge University Press, 2006

CHEM581 Wave function Analysis

Credits: 3

Pre-requisite: Knowledge in introductory quantum mechanics

Course Outline and Objective: Students are trained to extract various molecular properties and data from estimated wave functions, estimate electron density, bond order, and bond type, reactivity and many more.

Unit I Electron Partitioning Schemes (Basis-set based)

Introduction - Atomic charges – Bond Strength - Population Analysis – General classification – Basis-set based – Mulliken method, Lowdin method – Extension to Atom Bond energy partitioning (Special case of one-electron theory) - Hamilton method

Unit II Electron-Density Based Partitioning Schemes

Introduction – Atomic basins – Topology-based - Atoms in Molecules (AIM) method – Bond, Ring and Cage critical points – Applications - Physical-space partitioning by other methods Voronoi charges, Hirschfeld charges, Stewart charges, Generalized Atomic Polar Tensor (GAPT) method - Electron Localization Functions (ELF) – Role of Kinetic Energy in Bonding

Unit III Localized MO-based Partitioning

Localization of MOs - Schemes – Canonical vs Localized MOs – Natural Orbitals – Separation into Atomic Orbitals and Bond Orbitals - NBO analysis – Localization of core orbitals, Bonds and lone-pairs – Applications

Unit IV Energy-based Partitioning

Energy Decomposition Analysis (EDA) – Coulson's qualitative ideas - Morokuma-Kitaura (MK) Energy Decomposition – The Reduced Variational Space (RVS) Analysis – Comparisons – Extension of Coulson's model - Intermolecular Perturbation Theory (IMPT) – Fragment Molecular Orbital (FMO) based EDA – Applications – Electrostatic Potential Based analysis – Molecular electrostatic Potential (MEP)

Unit V Aromaticity Indicators

Introduction – Delocalization Indices - Topological Resonance Energy (TRE) - Harmonic Oscillator Model of Aromaticity (HOMA) - Nuclear Independent Chemical Shift (NICS)

References:

Introduction to Computational Chemistry, Frank Jensen, 3ed, Wiley, 2017

Encyclopaedia of computational chemistry, Ed. Paul von Rague Schleyer, John Wiley and Sons, 1998

Quantifying aromaticity with electron Delocalization measures, Chem. Soc. Rev., 2015, 44, 6434

Theoretical Aspects of Chemical Reactivity, Ed. A. Toro-Labbé, Elsevier, 2007, Chapter 5

CHEM582 Non-Equilibrium Thermodynamics

Credits: 3

Pre-requisite: CHEM313, CHEM324, CHEM414, CHEM571

Course Outline & Outcome: The course describes in a simple and practical way what non-equilibrium thermodynamics is and how it can add to science and engineering fields. It explains how to derive proper equations of transport from the second law of thermodynamics or the entropy production. The equations are frequently more precise than used so far, and can be used to understand the waste of energy resources in central process units in the industry. It introduces the entropy balance as an additional equation, to define the energy efficiency in energy conversion, create consistent thermodynamic models, and provide a systematic method for minimizing energy losses that are connected with transport of heat, mass, charge and momentum. It examines operation at the state of minimum entropy production, and proposed some rules of design for energy efficient operation.

Course Outcome: The goal is working knowledge about the description of irreversible processes. At the end of the course, the student should be able to explain

- the entropy production of a system with transport processes

- the coupled transport of heat, mass and charge

- the entropy production in a chemical reactor

- transport of heat and mass in a flow field

- the second law efficiency

- how the efficiency can be optimized in simple process equipment

Course Evaluation: Term paper: 25%, Oral Presentation: 25%, Assignments and Tests: 50%

Unit I Introduction to the problem

Development of irreversible processes – Definitions, Second law and open systems, Fluxes and chemically reactive systems, thermodynamic forces in spatially non-uniform systems – relation between flux and thermodynamic force, linear Onsager relations

Unit II Transport phenomena

Momentum transfer, Heat transfer, mass transfer; coupled processes; Fundamentals – Local equilibrium, balance equation and entropy production, Onsager's relation, Curie-Prigogine principle, minimum entropy production; Thermo-economics

Unit III Transport Processes: Diffusion – Maxwell Stefan equation, electrolyte systems, biological solutes in liquids; Heat and mass transfer – coupled heat and mass transfer, heat transport, coupling and coupled mass and energy balances, thermoelectric effects; Chemical Reactions – balance equation, dissipation of chemical reactions, reaction velocity, multiple chemical reactions, stationary states, biochemical reactions; Coupled systems of chemical reactions and transport processes; membrane transport

Textbook:

Valentin Parmon, Thermodynamics of non-equilibrium processes for Chemists with a particular application to catalysts, 1ed, Elsevier, 2010

Yasar Demirel, Non equilibrium thermodynamics Transport and rate processes in Physical, Chemical and Biological Systems, 3ed, Elsevier, 2014

Further Readings:

MIT Open course ware: https://ocw.tudelft.nl/courses/non-equilibrium-thermodynamics