# 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*


**Department of Chemistry**

**Tel** 91 413 2654 410
**Fax** 91 413 2656 740

Pondicherry University
Pondicherry 6050 014

https://chempu.ac.in
hod@chempu.ac.in

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# Department of Chemistry

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 21$^{st}$ 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

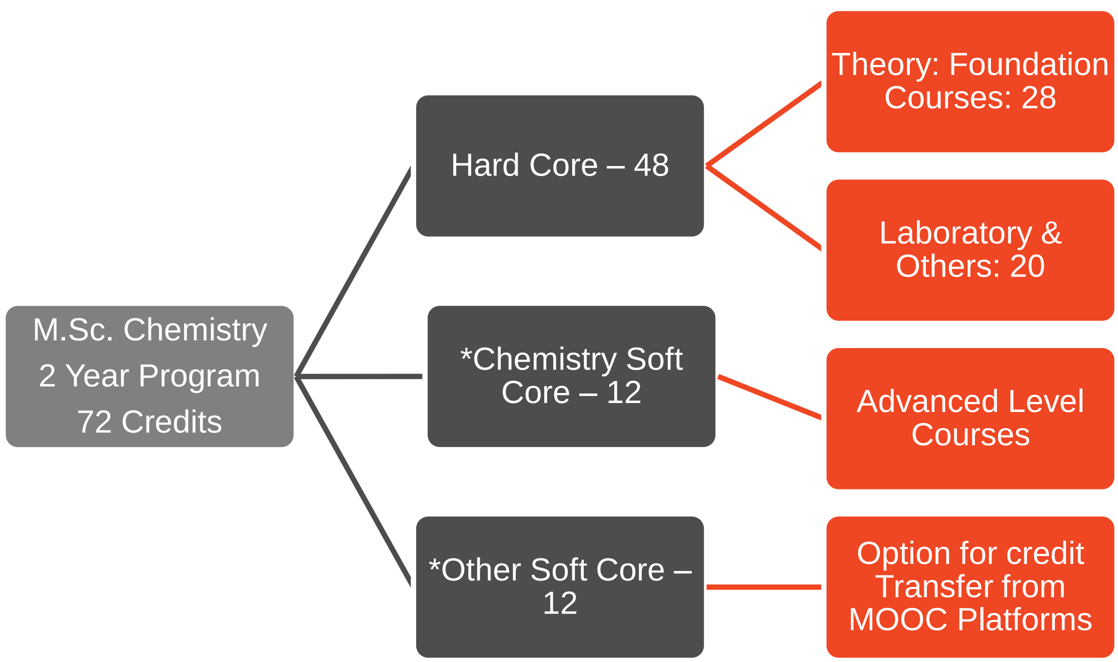
## *Lead and Collaborate*

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. Chemistry

The curriculum of Two-year M.Sc. Chemistry is spread over four 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 and rich educational experiences in diverse interdisciplinary and cross disciplinary domains. Course structure consists of foundational and advanced levels in chemistry and from other sciences with an emphasis to begin research from early stages.

CHART 1: Overview of M.Sc. Chemistry Curriculum




M.Sc. Chemistry

4 Semester
72 Credits
Graduate Research
Research Internships
Inter/cross disciplinary

* Options to mix & match courses to pursue pure chemistry or inter/cross disciplinary sciences

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

This two-year M.Sc. Chemistry program covers 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. Practical Training through summer internships, seminar and workshop participation, chemical industry and/or public sectors that involve chemical activities, are also involved.

Courses offered in the first two semesters aim at laying a strong foundation in professional chemistry education. Organization of course content 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 in the next two semesters. Students shall have the flexibility to choose 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 relevance and contemporary trends in research in those areas. Course tutor may include additional laboratory component within the credit points of the course.

Separate laboratory course credits are designed to equip the students with skills enabling them to enter a research-oriented career or industry or academic arena, on completing the program. In addition to developing experimental skills in chemistry, principles and tools of practicing eco-friendly chemistry, organizing, maintaining a chemistry laboratory, laboratory safety, micro-scale experiments, students develop hands-on experience with modern instruments and receive tutorial instructions from research scholars, post-doctorate researchers and visiting experts. Laboratory courses also inculcate ethics, values and competence in communication.

Components such as summer internship, seminar participation, project and comprehensive viva are opportunities offered to students to get wide-ranging experience in research and develop much needed career skills. Moreover, the proposed curriculum has the flexibility to include new programs with specialization in chemistry or programs of inter/cross disciplinary nature.

The rules and regulations of Choice Based Credit System (CBCS) are applicable to this program. Generally, a student takes four 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 two-year M.Sc. Chemistry program shall acquire a minimum of 72 credits in order to be eligible to receive the degree. The credit requirements are described in the later pages.

### 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: 72 Credits / 4 semesters
- Foundation Chemistry Courses: 48 Credits
- Advanced Chemistry Courses: 12 Credits
- Other Soft-Core Courses: 12 Credits
- Laboratory credits aimed at skill development
- Mandatory graduate research projects
- Flexibility to opt for pure chemistry or inter-disciplinary or cross-disciplinary curriculum
- Option for credit transfers from MOOC platform

## Credits Distribution

*M.Sc. Chemistry (4 semesters): 72 Credits*

Foundation Course Credits

Theory (9 courses, HC): 28

Laboratory (2 Courses, HC): 8

Advanced Course Credits

Research Project (2 Courses, HC): 8

Seminar + viva + Internship (HC): 4

Chemistry Courses

Theory (4 Courses, SC): 12

Other Soft-Core Credits

*Inter/Cross disciplinary (SC): 12

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

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

* Option is available for credit transfers from MOOC platforms

### Semester-wise Credits Distribution

The semester-wise credit assignments are only indicative in nature. Students shall register courses as and when they are offered and depending on availability of physical infrastructure. Courses offered for this program are of advanced in nature and require extended working hours. Most courses will have home-assignments, in-class problem solving sessions, tests, term-papers, seminar presentation, laboratory work etc. Therefore, students are advised to register and work on hard-core credits in accordance with their competence levels. Students are further advised to choose soft-core courses in terms of their long-term goals and their career options. Students shall complete the program within 8 semesters from their enrolment to the program.

Students shall have an option for credit transfers from MOOC platforms as Soft-Core credits. They are strongly advised to consult Faculty Advisor and SWAYM coordinator. The maximum number of credits shall be prescribed by the CBCS regulations and/or department program committee.

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. Course tutor shall have the option to prescribe his/her own evaluation method. However, the final grading will be awarded as per the CBCS regulations of the University.

*Semester 1 (20 Credits)*

CHEM410 Advanced Chemistry Laboratory I (3 Credits)

CHEM411: Symmetry & Structure (3 Credits)

CHEM412: Electronic Structure (3 Credits)

CHEM413: Chemical Bonding (2 Credits)

CHEM414: Chemical Reaction & Energetics (3 Credits)

CHEM415 Chemistry of main group Elements (3 Credits)

*Other Soft-Core Course (3 Credits)

*Semester 2 (22 Credits)*

CHEM420 Advanced Chemistry Laboratory II (3 Credits)

CHEM421: Reaction Kinetics & mechanism (4 Credits)

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

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

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

*Other Soft-Core Course (3 Credits)

*Semester 3 (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 4 (15 Credits)*

CHEM520 Research Project (4 Credits)

CHEM521 Seminar Participation and Review Writing (2 Credit)

Chemistry Soft-Core Courses (6 Credits)

*Other Soft-Core Courses (3 Credits)

*Option available to transfer credits from MOOC platform.

# Advanced Laboratory

This laboratory is designed to introduce research skills and prepare students for undertaking independent research project later in the program. 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 at least 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 one experiment in each of the three broad sub-domains of chemistry namely Inorganic, Organic and Physical/Computational together totaling to six experiments in CHEM410 and CHEM420 in two semesters.

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

*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