Syllabus

(M.Sc. in Chemistry under CBCS)

DEPARTMENT OF CHEMISTRY

GAUHATI UNIVERSITY

2016

Preface

The University Grants Commission has initiated several measures to bring in equity, efficiency and excellence in the Higher Education System of the country. These measures include enhancing academic standards and quality in higher education, innovation and improvements in curriculum, teaching-learning process, examination and evaluation system, besides governance and other matters.

In 2015, the UGC directed the Indian Universities to adopt the Choice Based Credit System (CBCS) in the undergraduate and post graduate level. The Choice-Based Credit System (CBCS) provides a 'cafeteria' type approach in which the students can take courses of their choice and learn at their own pace. It is now possible for students to undertake additional courses and acquire more than the required credits, and facilitates an interdisciplinary approach to learning.

In compliance with the UGC directives, Gauhati University began the process of implementing CBCS in the Post Graduate classes from the year 2016. Accordingly, the Department of Chemistry, Gauhati University revised and updated the Chemistry Syllabus for its Master of Science (M.Sc.) programme as per CBCS format, which is detailed herein. Under the present system, students admitted to this course, must have Major in Chemistry in the degree level with physics and Mathematics as part of their auxiliary subjects.

This syllabus for M.Sc. in Chemistry distributed over four semesters, and incorporates 24 courses with a total of 96 credits, and a minimum of 24 credits per semester. Detailed distribution of courses and the corresponding credits are given subsequently. Each semester provides for theory and practical courses, which could be identified as Core and Elective. For successfully completing the course, each student is required to complete 19 core courses and 5 elective courses.

The current system allows a student to choose elective courses, two in the third semester and three in the fourth semester. The Elective Courses offered by the Department in a particular semester may vary, depending on the requirements of the students, the intake capacity of the Department, and availability of expertise/resources required to successfully conduct a particular course.

The University also provides the students with the option of choosing between two types of elective courses, inter- and intra-departmental electives. The Department of Chemistry offers intra-departmental elective courses, in the third and fourth semesters. Here, the prospective student has to choose from set of courses which are being offered by the Department. In addition, the student is allowed to choose/opt for an inter-departmental course, termed as open-elective course, which will be offered by a Department other than the parent Department.

Following the spirit of CBCS, the Department can undertake measures to upgrade/update and modify course content in the current syllabus and introduce flexibility depending on the needs of the students.

Evaluation and grading under CBCS:

As already mentioned, a student is required to complete 24 credits in each semester, where 1 credit is equivalent to 1 contact hour per week (for theory) and 2 contact hours per week (for practical class). It is recommended that for end-semester examinations, the time allotted for 2 credit course is 2 hours; for 3 and/or 4 credit course(s), time allotted will be 3 hours.

The present system of evaluation requires 20% weightage to internal examination, based on the total mark equivalent for that course. The UGC recommends a 10-point grading system with the following letter grades as given below:

Table 1: Grades and Grade Points

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

A student obtaining Grade F shall be considered failed and will be required to reappear in the examination. For details on Examination, Assessment, grading and other modalities of CBCS system, students and the instructors are requested to consult GauhatiUniversity website link on CBCS (http://web.gauhati.ac.in/courses/cbcs/booklet)

DEPARTMENT OF CHEMISTRY: GAUHATI UNIVERSITY

Structure of M.Sc. Syllabus in Chemistry under CBCS

Total Credits: 96

Sl. No.	**Course Name**	**Nature of Course**	**Credits**
Semester I			**24**
CH101	Inorganic Chemistry 1	Core	3
CH102	Organic Chemistry 1	Core	3
CH103	Physical Chemistry 1	Core	3
CH104	Quantum Chemistry	Core	3
CH105	Spectroscopy 1	Core	3
CH106	Symmetry and Group Theory in Chemistry	Core	2
CH107	Laboratory Course I	Core	7
Semester II			**24**
CH201	Inorganic Chemistry 2	Core	4
CH202	Organic Chemistry 2	Core	4
CH203	Physical Chemistry 2	Core	4
CH204	Spectroscopy 2	Core	3
CH205	Green Chemistry	Core	2
CH206	Laboratory Course II	Core	7
Semester III			**24**
CH301	Biochemistry	Core	3
CH302	Modern Methods of Analysis	Core	3
CH303	Foundations of Organic Synthesis	Core	3
CH304	Seminar	Core	2
CH305	Laboratory Course III	Core	7
	Open 1	Elective	3
	Open 2	Elective	3
Semester IV			**24**
	Open 3	Elective	4
	Open 4	Elective	4
	Open 5	Elective	4
CH411	Project Dissertation	Elective	12

Elective courses to be offered in Semester III CH306. Solid State and Materials Chemistry CH307. X-ray Crystallography CH308. Environmental Chemistry CH309. Surface Science and Catalysis CH310. Food Chemistry (*These courses of interdisciplinary nature are also intended to be studied by students from other departments.*)	*Elective courses to be offered in Semester IV* CH401. Natural Products Chemistry CH402. Advanced Organic Synthesis CH403. Quantum and Computational Chemistry CH404. Catalysis Science & Technology CH405.Nanoscience& Nanotechnology CH406. Bioinorganic Chemistry CH407. Supramolecular Chemistry CH408. Organometallic Chemistry CH409. Medicinal Chemistry CH410. NMR Methods for Structure Elucidation

Note: Students in Semester IV may be offered a choice between Groups A, B or C, along with an elective from Group D.

Group A: CH401 (Natural Products Chemistry), CH402 (Organic Synthesis)

Group B: CH404 (Catalysis Science & Technology), CH405 (Nanoscience & Nanotechnology)

Group C: CH406 (Bioinorganic Chemistry), CH407 (Supramolecular Chemistry)

Group D: CH410 (NMR Methods for Structure Elucidation), CH403 (Quantum and Computational Chemistry), CH408 (Organometallic Chemistry), CH409 (Medicinal Chemistry)

Semester I
CH101: Inorganic Chemistry 1
Credits: 3 (45 h)

Course Objective: This is an introductory course on inorganic chemistry, through which students will appreciate the chemistry of the transition metals, aspects related tobonding, oxidation states and electronic/magnetic properties.

Learning outcome: Students will be able to explain/critically examine the chemistry of transition metals, structure and bonding.

1. **Descriptive Inorganic Chemistry (20 h)**
    - Structure and bonding in polyhedral boranes and carboranes, electron count in polyhedral boranes – styx numbering, Wade's rules – polyhedral skeletal electron pair theory (PSEPT), synthesis of polyhedral boranes. Metal borides.The hydroboration reaction, organoboranes including boronic acids, tetrahydridoborates – synthesis and synthetic use.Boron nitride, borazanes and borazines
    - Preparation and reactivity of lithium aluminium hydride; alkyl aluminium compounds; chemistry of Al, Ga, In and Tl in +1 and +2 oxidation states
    - Fullerenes and fullerides, nonmolecular compounds of carbon, different forms of silica, silicates, clays and zeolites; organo compounds of Si, Ge, Sn and Pb; phosphates, phosphazenes and phosphines; metal-oxo compounds, calixarenes, cryptands and crown ethers in complexation chemistry, metal chalcogenides, sulfur-nitrogen compounds
    - Organometallic compounds of Li, Be, Mg and Hg
    - Chemistry of the elements of the second and third transition series – general overview of compounds having the metals in their common oxidation states; halide containing clusters of niobium and tantalum; polyoxometallates of Mo and W; quadruple and quintuple M-M bonded compounds, methyltrioxorhenium (MTO); the Creutz-Taube complex; $RuCl_2(PPh_3)_3$; osmium tetroxide; Vaska's compound; palladium complexes in the oxidation state 0; Pt(II,IV) linear chain compounds.

2. **Introduction to Solid State Chemistry (10 h)**
    - Structure of simple solids – metals, alloys and compounds; common structure types. Synthesis of solid state compounds - ceramic method, hydrothermal synthesis, CVD and intercalation methods. Characterization of solids.
    - Bonding in solids –free-electron and band theory of solids.
    - Properties of solids – optical, magnetic and electrical properties of solids.

3. **Organometallic Chemistry (15 h)**
    - Synthesis, structure, bonding and reactivity of mono and polynuclear metal carbonyls. Substituted metal carbonyls.Vibrational spectra of metal carbonyls.
    - Types of M-C bonds, synthesis and reactivity of metal alkyls, carbenes, alkenes, alkynes, and arene complexes; metallocenes and bent metallocenes.
    - Reactions of organometallic complexes: substitution, oxidative addition, reductive elimination, insertion and deinsertion; catalysis - hydrogenation, hydroformylation, Monsanto process, Wacker process, alkene polymerization,olefin metathesis, Suzuki coupling reaction.

Books Recommended

1. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann; Advanced Inorganic Chemistry, 6th ed. Wiley, 1999
2. P.W. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong; Shriver & Atkins' Inorganic Chemistry, 5th ed. Oxford University Press, 2010.
3. Fundamental Concepts of Inorganic Chemistry, Vols. 1-7, by A.K. Das and M. Das, CBS Publishers and Distributors, 2015
4. L. Smart, E. Moore, Solid State Chemistry: An Introduction, 2nd Ed. Nelson Thorns Ltd. 2004.
5. A. R. West, Solid State Chemistry and Its Application, Wiley Student Edition, John Wiley & Sons. 1998.
6. R. H. Crabtree, Organometallic Chemistry of the Transition Metals 2nd Ed. , John Wiley, 1993.
7. C.Elschenbroich, A. Salzer, Organometallics: A Concise Introduction, 2nd Ed. Wiley VCH, 1995.

Semester I
CH102: Organic Chemistry 1
Credits: 3 (45 h)

Course objective: Students will be introduced to the concepts of reaction mechanism, reaction intermediates and stereochemistry.

Learning outcome: Students will be able to appreciate/demonstrate/explain the unique features of organic reactions mechanism, reaction intermediates and stereochemistry, and solve related problems.

1. **Kinetics and Energetics of Reaction Mechanism (13h)**
   - TST theory of reaction rates: kinetics & thermodynamics of activation. Reaction profiles for multistep reactions, Hammond postulate, Curtin-Hammett Principle; kinetic and thermodynamic control.
   - Linear free energy relationships (LFER): Hammett equation - substituent and reaction constants; the Taft treatment of polar and steric effects in aliphatic compounds; kinetic isotope effects in organic reactions.
   - Effects of conformation on reactivity: anomeric effect, stereoelectronic effects, neighbouring group participation.

2. **Reaction Mechanisms & Intermediates: Structure & Reactivity I (12h)**
   - Carbanions: enolates and enamines, Kinetic and thermodynamic enolates, lithium and boron enolates in aldol and Michael reactions, alkylation and acylation of enolates; name reactions under carbanion chemistry - Claisen, Dieckmann, Knoevenegal, Stobbe, Darzen, Acyloin condensations, Shapiro reaction, Julia olefination, Brook rearrangement,Sakurai reaction,Henry reaction,Kulinkovichreaction,Nefreaction,Baylis-Hillman reaction
   - Ylids: Chemistry of phosphorous and sulfur ylids - Wittig and related reactions, Peterson olefination
   - Carbocation: structure and stability of carbocations, classical and non-classical carbocations, neighbouring group participation and rearrangements including Wagner-Meerwein, pinacol-pinacolone, semi-pinacol rearrangement, C-C bond formation involving carbocations, oxymercuration, halo-lactonisation,Tishchenko reaction,Ritter reaction,Prins reaction.

3. **Reaction Mechanisms &Intermediates: Structure & Reactivity II (10 h)**
   - Carbenes and Nitrenes: Structure of carbenes, generation of carbenes, addition and insertion reactions, rearrangement reactions of carbenes such as Wolff rearrangement, generation and reactions of ylids by carbenoid decomposition (existence of O and N based ylids), Structure of nitrene, generation and reactions of nitrene and related electron deficient nitrogen intermediates, Curtius, Hoffmann, Schmidt, Beckmann rearrangement, Tebbeolefination reactions.
   - Radicals: Generation of radical intermediates and its (a) addition to alkenes, alkynes (inter &intramolecular) for C-C bond formation and Baldwin's rules (b) fragmentation and rearrangements. Name reactions involving radical intermediates such as Barton deoxygenation and decarboxylation, McMurry coupling.

4. **Stereochemistry (10h)**
   - Classification of organic molecules into different Point Groups, R/S, E/Z nomenclature in C, N, S, P containing compounds; concept of absolute and relative configuration; chirality in molecules devoid of chiral centers- allenes, spiranes and biphenyls (atropisomerism).
   - Concepts of stereogenic center – chirotopic and achirotopic center; homotopic and heterotopic ligands and faces (prostereoisomerism and prochiralityetc); optical purity and enantiomeric excess; conformation of acyclic organic molecules, cyclohexane and decalins.

Books Recommended

1. F. A. Cary and R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edition, Springer, 2009.
2. A. J. Kirby, Stereoelectronic Effects, 1st edition, OUP
3. T. H. Lowry, K. S. Richardson, Mechanism and Theory in Organic Chemistry.
4. J. Clayden, N. Greeves, S. Warren, Organic Chemistry, 2nd edition, OUP 2012
5. E. V. Anslyn, D. A. Dougherty, Modern Physical Organic Chemistry, University Science Books, 2005
6. E.L. Eliel, S. H. Wilen, Stereochemistry of Organic Compounds

Semester I
CH103: Physical Chemistry 1
Credits: 3 (45 h)

Course objective: Students will be introduced to equilibrium and non-equilibrium thermodynamics, statistical mechanics, polymer chemistry. Basic aspects of sampling methods and dataanalysis will also be covered.

Learning outcomes:Students will be able to explain the fundamentals of equilibrium and non-equilibrium thermodynamics, statistical mechanics, polymer chemistry and apply the concepts to solving problems.

1. Equilibrium and Non-equilibrium Thermodynamics (18 h)

- Laws of thermodynamics, state and path functions and their applications, Maxwell's relations; spontaneity and equilibria; Le Chatelier principle
- Non-ideal system: thermodynamics of real gases and gas mixtures, fugacity and its determination, non-ideal solutions, activity and activity coefficient-different scales of activity coefficient, electronic activity coefficients
- Phase equilibrium: thermodynamic criteria of phase equilibrium, Gibbs phase rule and its application to three component systems- triangular plots- water- acetic acid –chloroform system, ammonium chloride-ammonium sulphate-water system
- Non-equilibrium thermodynamics: forced flows and entropy of production, coupled flows and phenomenological relations, Onsager reciprocal relations, thermodynamic effects- Seebeck and Peltier and Thomson effect

2. Statistical Thermodynamics (15 h)

- Statistical mechanics of systems independent particles: Maxwell Boltzmann distribution, entropy and probability. Calculation of thermodynamic properties for independent particles,- molecular partition functions- evaluation of translational, rotational and vibrational and nuclear partition functions
- Thermodynamic properties of monatomic and diatomic gases (Suckur-Tetrode equation)- calculation of partition functions, thermodynamic function, principles of equipartition, heat capacities (Einstein model and Debye modification), residual entropy, equilibrium constant

3. Polymer Chemistry (6 h)

- Molecular weight of polymers, determination of molecular weight, kinetics of polymerization reaction, copolymerization, average dimension of polymer molecules, size exclusion chromatography

4. Sampling and Data Analysis: (6 h)

- Sampling of solid, liquid and gaseous samples, mean and standard deviation, absolute and relative errors, linear regression, covariance and correlation coefficient

Books Recommended

1. P. Atkins, J. Paula, Physical Chemistry, 9th Edition, Oxford University Press, Oxford 2010.
2. I. R. Levine, Physical chemistry, 6th Edition, Mcgraw Hill Education, 2011.
3. D. A. McQuarrie, J. D. Simon, Physical Chemistry: A Molecular Approach, Viva Student Edition, 1st Edition, 2011.
4. R. S. Berry, S. A. Rice and J. Ross, Physical Chemistry, 2nd Edition, Oxford University Press, Oxford 2007.
5. D. A. McQuarrie, Statistical Mechanics, University Science Books, California, 2005.
6. J. Mendham, R. C. Denney, J. D. Barnes, M. Thomas, B. Sivasankar, Vogel's Textbook of Quantitative Chemical Analysis, 6th Edition, Pearson, 2009.
7. V. R. Gowarikar, N. V. Viwanathan, J. Sreedhar, Polymer Science, 1st Edition, New age International Publishers, 1986.
8. G. Odian, Principles of Polymerization, 4th Edition, Willy Student Edition, 2004.

Semester I
CH104: Quantum Chemistry
Credits: 3 (45 h)

Course objective: To introduce students to the fundamental principles and modern aspects of quantum chemistry.

Learning outcome: Students will be able to explain the theoretical basis of quantum chemistry, and critically examine/interpret the theories/principles. Students will be able to compare various approximate formalisms and their validity in explaining experimental phenomena.

1. **Wavepackets and Operators (15 h)**
   - Black-body radiation, the photoelectric and Compton effects, atomic spectra, the duality of matter, Dirac bra-ket notation, review of vectors and vector spaces
   - Hermitian operators, matrix elements, The diagonalization of the Hamiltonian, wave-packets, wave functions of one particle and many particles system, the equation for the wave function, the separation of the Schrodinger equation,
   - Born interpretation, expectation values of observable properties, complementarity and complementary observable, uncertainty principle, general angular momentum operators, step-up and step-down operators, theoretical basis of the L-S and J-J coupling schemes.

2. **Solution of Eigenvalue Equations (10 h)**
   - Solutions of the energy eigenvalue equations for particles in a ring, Rigid Rotor, The angular momentum, QM treatment of H-atom
   - QM treatment of Harmonic Oscillator, Free electron MO theory of benzene; HMO treatment for unsaturated carbon compounds, extended Hückel Theory, elements of band theory.

3. **Approximate Methods(10 h)**
   - Time-independent perturbation theory of a two level system (up to second order), the first order correction to the energy and wave function, perturbation theory for degenerate states, the second order correction to the energy, time dependent behaviour of a two level system, the Rabi formula, the effect of a slowly switched constant perturbation, the variation theorem, linear variation function-secular equation, the Rayleigh ratio.

4. **Born-Oppenheimer Approximation (10 h)**
   - Born-Oppenheimer approximation, product wave-functions, complete many electron wave functions including electron spin, Pauli's anti-symmetry and exclusion principles, Singlet and triplet states, central field model of many electron atoms (He atom), Slater type orbitals, splitting of term energies in presence of electric and magnetic field (Stark effect and Zeeman effect)

Books Recommended

1. P. Atkins, R. Friedman, Molecular quantum Mechanics, 4th Edition, Oxford University Press, Oxford 2008.
2. I. N. Levine, Quantum Chemistry, 7th Edition, PHI Learning Pvt. Ltd., 2014.
3. David J. Griffiths, Introduction to Quantum mechanics, 2nd edition, Pearson Education Ltd., 2014
4. A. Szaboo, N. S. Ostlund, Modern Quantum Chemistry, 1st edition (Revised), 2015.

Semester I
CH105: Spectroscopy 1
Credits: 3 (45 h)

Course objective: Students will be introduced to the fundamental principles of spectroscopy with special emphasis on the rotational, vibrational and electronic spectroscopies.

Learning outcome: Students will be able to identify/explain the theoretical basis of different spectroscopic techniques, and show their application in analyzing/interpreting experimental data.

1. **Introduction (5 h)**
   - Fundamental aspects of absorption and emission spectroscopy. Probability of transition, oscillator strength, dipole strength. Spontaneous and stimulated emission. Origin of selection rules using symmetry. Quantitative treatment of Fourier Transform spectroscopy.

2. **Rotational, Vibrational and Raman Spectroscopy (24 h)**
   - Rotational spectroscopy. Classification of molecules based on their moment of inertia, rotational energy levels, molecular geometry determination, stark effect, molecular dipole moment. Rotational spectroscopy of symmetric and asymmetric top molecules.
   - Vibrational spectroscopy: Harmonic and anharmonic oscillators. Morse potential, mechanical and electrical nharmonicity, selection rules. The determination of anharmoncity constant and equilibrium vibrational frequency from fundamental and overtones. Vibrational selection rules using symmetry, polarization of transitions. Normal modes analysis using group theory.
   - Raman spectroscopy- polarizability tensor, Stokes and anti-Stokes lines, Origin of characteristic bands, instrumentation and applications in chemical and biological systems.
   - Infrared and Raman spectroscopy of simple inorganic and organic molecules, predicting number of active modes of vibrations, organic functional group identification through IR spectroscopy, analysis of representative spectra of metal complexes with various functional groups at the coordination sites; application of isotopic substitution.

3. **Electronic Spectroscopy and CD/ORD (16 h)**
   - UV-visible spectroscopy: Electronic transitions, Franck-Condon principle, vertical transitions; Selection rules, parity, symmetry and spin selection rules. Instrumentation, Application in organic structure analysis; polarization of transitions
   - Fluorescence and phosphorescence spectroscopy: Jablonski Diagram, origin of fluorescence and phosphorescence processes, quantum yield, fluorescence quenching-static and dynamic. Instrumentation and applications
   - CD/ORD & MCD: Polarised light, definition, deduction of absolute configuration, octant rule for ketones. Instrumentation and illustrative applications

Books Recommended

1. J. M. Hollas, Modern Spectroscopy, John Wiley & Sons, 4th Ed., 2004
2. D.L. Pavia, G. M. Lampman, G. S. Kriz, Introduction to Spectroscopy, 4th Ed.,Cengage, 2001
3. R. S. Drago, Physical Methods in Chemistry, 1992
4. R. M Silverstein, F. X. Webster, D. J. Kiemle, D. L. Bryce, Spectrometric Identifications of Organic Compounds, 8th Edition, Wiley India Pvt. Ltd, 2015.
5. B. Valuer, Molecular Fluorescence, Wiley-VCH, 2002
6. J R Lakowicz, Principles of Fluorescence Spectroscopy, Springer, 3rd Edn, 2006

Semester I
CH106:Symmetry and Group Theory in Chemistry
Credits: 2 (30h)

Course objective: Students will be able to recognize and understand the importance of group theory molecular and crystallographic symmetry, in molecular structure and bonding.

Learning outcome: Students will be able to explain/describe/rationalize molecular structure and bonding using group theory.

1. **Groups and Matrices(2 h)**
   - Definitions and elements of group theory and matrix algebra

2. **Molecular Symmetry and the Symmetry Groups(4 h)**
   - Symmetry elements and operations, classes of symmetry operations, symmetry and chirality, symmetry point groups, symmetry of the Platonic solids

3. **Representation of Groups(6 h)**
   - Matrix notation for geometric transformations, reducible and irreducible representations, rules about irreducible representation as derived from great orthogonality theorem, relationship between reducible and irreducible groups, character tables

4. **Chemical Applications of Group Theory(12 h)**
   - Group Theory and Quantum Mechanics - wave functions as bases for irreducible representations, the direct product and its importance in predicting spectral transition probabilities.
   - Molecular vibrations - symmetry of normal vibrations, selection rules for fundamental vibrational (IR and Raman) transitions.
   - Symmetry properties of atomic orbitals, molecular orbitals for σ and π bonding in AB_4 molecules, MO treatment of the bonding in ferrocene. Ligand field states, construction of the correlation diagram for the d^2 configuration in an octahedral environment.

5. **Crystallographic Symmetry (6 h)**
   - Translational and point symmetry elements in crystal symmetry, glide planes and screw axes, the crystal systems, Bravais lattices, crystallographic point groups, space groups.

BooksRecommended

1. F. A. Cotton, Chemical Applications of Group Theory, 3rd Edition, Willey India Pvt. Ltd. 2008.
2. R. L. Carter, Molecular Symmetry and Group Theory, John Wiley & Sons, 1998

Semester I
CH107: Practical Organic Chemistry
Credits: 7

Course objective: Students will be introduced to common laboratory practices, techniques/apparatus for carrying out a synthesis, isolation & extraction of natural products, and quantitative estimation/characterization.

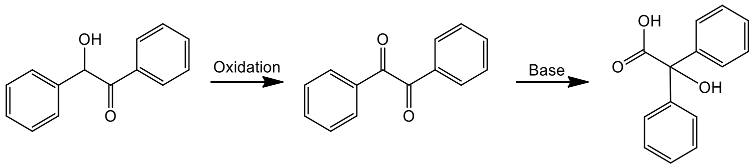
Learning outcome: Students will be able to perform qualitative and quantitative analysis of organic compounds and mixtures, implement multi-step organic synthesis and operate common/sophisticated instruments.

1. **Qualitative analysis** : Binary mixture analysis (solid-solid, solid-liquid, liquid-liquid)

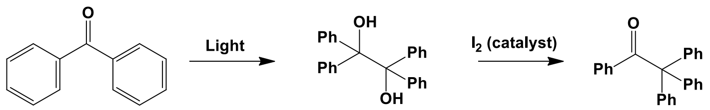
2. **Chromatography experiments** :
   - Qualitative TLC separation and identification
   - Column chromatographic separation of a mixture of compounds.

3. **Synthesis (2-steps)** :

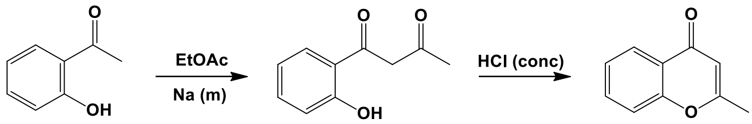
   - (Benzoin – Benzil – Benzilic acid) : Base catalysed, rearrangement



   - (Benzophenone – Benzopinacol – benzopinacolone) : Photochemical, rearrangement



   - (2-Hydroxyacetophenone – 1,3-diketone – Chromone) : Acid catalysed cyclisation



   - Solvent free reductive amination: Synthesis of imine from aldehyde and amine in solvent free condition and its reduction to amine using $NaBH_4$.
   - Oxidation of phenanthrene to phenanthrene-dione and its subsequent condensation to imidazophenanthrene derivative.
   - Multicomponent reaction of aldehyde, β−keto ester and urea/thiourea for the synthesis of dihydro-pyrimidine derivatives (Biginelli reaction)
   - Multicomponent reaction of aldehyde, β-keto ester and ammonia for the synthesis of dihydro-pyridine derivatives (Hantzsch Pyridine Synthesis)

4. **Experiments on Natural products:**

   - Introduction to extraction and phytochemical screening/analysis of Natural Products (A case study).
   - Extraction of carotenoids from a natural source.
   - Isolation of (−)-Menthol from Peppermint Oil.
   - Saponification of Vegetable Oil
   - Conversion of Vegetable Oil to Biodiesel.

5. **Quantitative analysis** :

   - Estimation of amino acids using titrimetric methods
   - Estimation of sugars using titrimetric (redox) methods.

- Spectroscopic methods for estimation of functional groups.
- Estimating the formation/stoichiometry of donor-acceptor complex involving anthracene and picric acid (Job's method).
- Determination of quantum yield of a chromophore/dye in a particular solvent.
- Chiral resolution of a racemic mixture by crystallisation and determination of enantiomeric excess.

Books Recommended:

1. B. S. Furniss, A. J. Hannaford, P. W. G. Smith, Vogel's Textbook of Practical Organic Chemistry, Pearson, 2012.
2. V. K. Ahluwalia, S. Dhingra, Comprehensive Practical Organic Chemistry, University Press.
3. F. G. Mann, B. C. Saunders, Practical Organic Chemistry, 3^{rd} Edition Longman, 1978
4. Selected articles from *Journal of Chemical Education*, ACS Publications.

Semester II
CH201: Inorganic Chemistry 2
Credits: 4 (60 h)

Course objective: Introduction to non-transition elements chemistry, including basic organometallic chemistry. Introductory ideas of solid states, and inorganic reaction mechanism and photochemistry

Learning outcome: Students will be able to apply their knowledge of inorganic and solid state chemistry in explaining, interpreting and critically examining bonding/structure/reactivity of metal complexes and organometallic compounds.

1. **Bonding in Inorganic and Coordination Compounds (15h)**
    - VBT (hybridization), CFT and their limitations; ligand field theory, d-orbital wave functions, d-orbital splitting in octahedral, square planar, square pyramidal, trigonalbipyramidal, and tetrahedral complexes; Jahn-Teller distortion, CFSE for d^1 to d^{10} systems, pairing energy, low-spin and high-spin complexes;, and molecular orbital (MO) theory of selected octahedral, tetrahedral complexes and other geometries, Walsh Diagram.

2. **Electronic Spectra ofTransition Metal Complexes (10 h)**
    - *d-d* transition, charge transfer transition, color, intensity and origin of spectra, interpretation, term symbols and splitting of terms different geometries, selection rules for electronic transitions, correlation, Tanabe-Sugano and Orgeldiagrams, calculation of Dq, B and C, nephelauxetic ratio.

3. **Magnetic Properties (10 h)**
    - Magnetic properties of free ions, types of magnetic behaviour: dia-, para-, ferro- and antiferro-magnetism, temperature independent paramagnetism, magnetic susceptibility - Van Vleck equation, experimental measurement, magnetic moment - orbital contribution, quenching of contribution, effect of spin orbit coupling, spincrossover. Temperature dependence of magnetic susceptibility, exchange coupling effects. Magnetic properties of second and third transition series and lanthanides.

4. **Mechanism of Inorganic Reactions(9 h)**
    - Substitution in octahedral and square planar complexes. Lability, trans-effect, conjugate base mechanism, racemisation, electron transfer reactions: inertness and lability, inner sphere and outer sphere mechanism, Marcus theory.

5. **Inorganic Photochemistry(6 h)**
    - Photosubstitution and photoredox reactions of chromium, cobalt and ruthenium compounds, Ligand field and charge transfer state (Thexi& DOSENCO states), cis-trans isomerization, photocatalysis and solar energy conversion by ruthenium complexes.

6. **Nuclear and Radiochemistry (10 h)**
    - Radioactive decay processes, Fermi theory, half-lives, auger effect. Nuclear reactions – notations, comparison with chemical reaction: Types of nuclear reactions. Applications of radioisotopes as tracers (activation and isotope dilution analysis).Age determination, radiolysis of water, units for measuring radiation absorbed by matter, radiation dosimetry.Radiation induced chemistry–sources of radiation, chemical effects produced by the absorption of ionizing radiation and high energy ions and electrons from accelerators - radiation induced synthesis of materials.

Books Recommended:

1. J. E. Huheey, E. A. Keiter and R. L. Keiter; Inorganic Chemistry: Principles of Structure and Reactivity, 4th Ed. Pearson Education, 2006.
2. B. N. Figgis, M. A. Hitchman; Ligand Field theory and its Applications, Wiley India, 2010.
3. G. L. Miessler, D Tarr; Inorganic Chemistry. 3rd Ed., Pearson Education, 2004.
4. P. W. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong; Shriver & Atkins' Inorganic Chemistry, 5th Ed. Oxford University Press, 2010.
5. Fundamental Concepts of Inorganic Chemistry, Vols. 1-7, by A.K. Das and M. Das, CBS Publishers and Distributors, 2015.
6. R. L. Dutta, A. Syamal, Elements of Magnetochemistry, 2nd Ed. Affiliated East-West Press Pvt. Ltd.-New Delhi, 2004.
7. F. E. Mabbs, D. J. Machin, Magnetism and Transition Metal Complexes, Dover Pub. Inc., 2008.
8. Reaction Mechanism in Inorganic Chemistry 2nd Ed. R. R. Jordan Oxford University Press, 1998.
9. F. Basolo, R. G. Pearson, Mechanism of Inorganic Reactions 2nd Ed. Wiley Eastern Pvt. Ltd. 1973.
10. D. M. Roundhill, Photochemistry and Photophysics of Metal Complexes; Plenum: New York, 1994.
11. 'Photochemical Processes' in Volume 1, Chapter 7.3 of Comprehensive Coordination Chemistry, G. Wilkinson (Editor-in-Chief), Pergamon Press, 1987.
12. H.J. Arnikar, Essentials of Nuclear Chemistry, 4th Ed. Wiley Eastern, New Delhi, 1995.
13. G. Friedlander, J.W. Kennedy, E. S. Macias, and J. M. Miller, Nuclear & Radiochemistry, 3rd Edition John Wiley, New York. 1981.

Semester II
CH202: Organic Chemistry 2
Credits: 4 (60 h)

Course objective: The objective of the course is to educate students on the various types of organic reactions, their mechanisms and applications.

Learning outcome: On the completion of the course students will acquire the detailed knowledge on photochemical, pericyclic, oxidation and reduction reactions.

1. **Organic Photochemistry (15 h)**
   - Introduction to organic photochemical-photophysical processes, chemiluminescence, photosensitization
   - Photochemistry of carbonyl compounds: α-cleavage, β-cleavage, intramolecular H-abstraction, addition to π-systems-Paterno-Buchi reaction; Photochemistry of olefins - photostereomutation of cis-trans isomers, optical pumping, cycloaddition, photochemistry of conjugated polyenes, photochemistry of vision
   - Photochemistry of enones; Photo-rearrangement reactions, di-π-methane rearrangement, Photo-rearrangement of cyclohexadienones, Barton rearrangement; Singlet oxygen photochemistry

2. **Oxidation Reactions (12 h)**
   - Metal based and non-metal based oxidations (Cr, Mn, Al, Ag, Os, Ru, Se, DMSO, hypervalent iodine and TEMPO based reagents). Reagents (Fremy’s salt, silver carbonate, peroxides/per-acids);
   - Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation, Sharpless asymmetric dihydroxylation, Baeyer-Villiger oxidation, Wacker oxidation, hydroboration-oxidation, Prevost reaction and Woodward modification.

3. **Reduction Reactions (15 h)**
   - Catalytic hydrogenation (Pd/Pt/Rh/Ni). Wilkinson catalyst, Noyori asymmetric hydrogenation;
   - Metal based reductions using Li/Na/Ca in liquid ammonia, Sodium, Magnesium, Zinc, Titanium and Samarium (Birch, Pinacol formation, McMurry, Acyloin formation, dehalogenation and deoxygenations);
   - Hydride transfer reagents from Group III and Group IV in reductions (NaBH4 triacetoxyborohydride, L-selectride, K-selectride, Luche reduction, LiAlH4, DIBAL-H, and Red-Al, Trialkylsilanes and Trialkylstannane, Meerwein-Pondorff-Verley reduction);
   - Stereo/enantioselective reductions (Chiral Boranes, Corey-Bakshi-Shibata).

4. **Pericyclic Reactions (18 h)**
   - MO symmetry, FMO of conjugated polyenes. Woodward-Hoffmann principle of conservation of orbital symmetry, allowed and forbidden reactions, stereochemistry of pericyclic reactions, orbital symmetry correlation method, PMO method.
   - Cycloaddition reactions: 2+2, 4+2, 6+2 cycloadditions, 3+2 and 4+3 dipolar cycloadditions; stereoselectivity of the reactions, regioselectivity of 4+2 cycloaddition reaction.
   - Sigmatropic rearrangement: (m+n) sigmatropic rearrangement of hydrogen and chiral alkyl groups; Divinylcyclopropane rearrangement, fluxional molecules, stereoselectivity in Cope and Claisen rearrangement. Sommelet-Hauser rearrangement.
   - Electrocyclic reactions and cycloreversions: Conrotatory and disrotatory process, Stereoselectivity of the reactions.
   - Linear and nonlinear cheletropic rearrangement, theories of cheletropic reactions, stereoselectivity of the reactions.
   - Ene reactions: of 1,7-dienes, carbonyl enophiles, simple problems. Claisen rearrangement and its variants, aza-Cope rearrangement (Overman rearrangement), ene reaction (metallo-ene; Coniaene).

Books Recommended

1. F. A. Cary, R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edition, Springer, 2009.
2. M. B. Smith, Organic Synthesis, 2nd Edition, 2005
3. W. Carruthers and I. Coldham, Modern Methods of Organic Synthesis, First South Asian Edition 2005, Cambridge University Press.
4. J. Clayden, N. Greeves, S. Warren, Organic Chemistry, 2nd edition, OUP 2012
5. E. V. Anslyn, D. A. Dougherty, Modern Physical Organic Chemistry, University Science Books, 2005

Semester II
CH203: Physical Chemistry 2
Credits: 4 (60 h)

Course objective: Students will be introduced to the concepts of chemical kinetics, electrochemistry, molecular dynamics and fast reaction kinetics.

Learning outcome: Students will able to describe/examine the concepts and theories of chemical kinetics and electrochemistry, and the applications of molecular dynamics, fast reactions and energy storage.

1. **Chemical Kinetics (8 h)**
   - Steady state approximation and its applications, Oscillating reactions, chemical Chaos, Belousov-Zhabotinski reaction, straight-chain reaction-hydrogen halogen reactions, alkane pyrolysis, Branching-chain reactions- the hydrogen-oxygen reaction, explosion limits, Enzyme catalyzed reactions, Michaelis-Menten mechanism- Lineweaver-Burk and Eadie plots, enzymeinhibiton.

2. **Molecular Reaction Dynamics (8 h)**
   - Collisions of real molecules- trajectory calculations, Laser techniques, reactions in molecular beam, -reaction dynamics, Estimation of activation energy and calculation of potential energy surface- the transition state theory (TST) of bimolecular gaseous reactions, statistical and thermodynamic formulations. Comparison between TST and hard sphere collision theory, Theory of unimolecular reactions- Lindemann theory and its limitations, kinetics of reactions in solution- diffusion controlled and chemically controlled reactions, TST of reactions in solution- Bronsted and Bjerrum equation, effect of ionic strength, kinetic salt effect.

3. **Study of Fast Reactions (8 h)**
   - Stopped flow technique, temperature and pressure jump methods, NMR studies in fast reactions, shock tube kinetics, relaxation kinetics, Linearized rate equation, relaxation time in single step fast reactions, determination of relaxation time.

4. **Theories of Unimolecular Reactions (6 h)**
   - Drawbacks of Lindemann theory- Hinselwood modification, RRK theory, slaters treatment, RRKM theory.

5. **Dynamic Electrochemistry (8 h)**
   - Ion-solvent interaction- the Born model, Thermodynamic parameters of ion solvent interactions- structural treatment, the ion-dipole model-its modifications, ion-quadrupole and ion-induced dipole interactions, Primary solution- determination of hydration number, compressibility method and viscosity-mobility method, Debye-Huckel theory of ion-ion interactions- derivation, validity and limitations, extended Debye-Huckel-Onsager equation. The random walk model of ionic diffusion- Einstein Smoluchowski reaction.

6. **Theories of Electrical Interface: (6 h)**
   - Electrocapillary phenomena- Lippmann equation, electron transfer at interfaces, polarizable and non-polarizable and nonpolaisable interfaces, Butler-Volmer equation, Tafel plot

7. **Electro-analytical Techniques: (10 h)**
   - Potential step methods, potential sweep methods, Polarography and Pulse voltammetry. Controlled current techniques, Techniques based on impedance.

8. **Systems forElectro-chemical Energy Storage & Conversion: (6 h)**
   - Batteries: Types of Batteries, Lead- acid batteries, Nickel-cadmium batteries and Li-ion batteries, Supercapacitors: Electrical double layer capacitor, Pseudo-capacitor, Fuel Cells

Books Recommended

1. P. Atkins and J. Paula, Physical Chemistry, 9th Edition, Oxford University Press, Oxford 2010.
2. I. R. Levine, Physical chemistry, 6th Edition, Mcgraw Hill Education, 2011.
3. K. J. Laidler, Chemical Kinetics,3rd Edition, Pearson, 2012.
4. J. O. Bockris, A. K. N. Reddy, Modern Electrochemistry Part 1, 2A and 2B, 2nd Edition, Springer
5. A. J. Bard, L. R. Faulkner, Electrochemical Methods Fundamentals and Applications, 2nd edition, Willy India, 2006.

Semester II
CH204: Spectroscopy 2
Credits: 3 (45 h)

Course Objective: Core course on spectroscopy, aimed at introducing students to the fundamental principles of NMR, ESR, Mössbauer spectroscopy and Mass spectrometry, with emphasis on application. Mössbauer spectroscopy will be dealt on an introductory level with selected examples.

Learning outcome: Students will be able to explain the basic working principle of magnetic resonance and mass spectroscopic techniques and their application in chemistry analysis.

1. **NMR Spectroscopy (22h)**
   - NMR phenomenon, Zeeman splitting, factors affecting sensitivity and resolution of a NMR spectrum, chemical shift tensor,^{1}H NMR-inductive and anisotropic effects on chemical shifts (δ), chemical and magnetic equivalence.First order patterns- δ and J to structural correlations.Second order effects in AB, AX and ABX spin systems, simplification of second order spectrum using high magnetic field. ^{13}CNMR (DEPT) and ^{13}Cδ to structural correlations, Satellites.
   - Pulse and Fourier transformation in NMR. Introduction to 2D NMR (COSY, HSQC).T_1, T_2 and NOE.
   - Dynamic processes by VT NMR- restricted rotation (DMF,annulenes and related systems), ring inversion(cyclohexane), degenerate rearrangement (bullvalene) and fluxional inorganic molecules, fluxionality in organolithium compounds in solution. Derivation of activation energies and thermodynamic parameters from dynamic processes,
   - NQR spectroscopy:Principles and applications.
   - NMR of Si, F, Xe, B, Li and P nuclei. NMR ofparamagnetic metal complexes-contact and pseudo-contact shifts; magnetic moment measurement. Introduction to solid-state NMR–CP MAS.

2. **ESR Spectroscopy (10 h)**
   - ESR spectra of organic and inorganic compounds, ZFS, Kramer's degeneracy, determination of electronic structure, Zeeman splitting, g-values, hyperfine and super hyperfine coupling constants, practical considerations of measurements, and instrumentation

3. **Mass Spectrometry (8h)**
   - Mass spectrometry: basic principles, ionization techniques, isotope abundance, molecular ion, fragmentation processes of organic molecules, deduction of structure through mass spectral fragmentation. ESI-MS and MALDI-MS-applications in biomolecules. Studies of inorganic/coordination and organometallic representative compounds. Instrumentation

4. **Mössbauer spectroscopy(5h)**
   - Principles, instrumentation and applications.

Books Recommended

1. C.N. Banwell, E. M. McCash, Fundamentals of Molecular Spectroscopy, 4th Edition, Tata McGraw Hill, 1994.
2. D.L. Pavia, G. M. Lampman, G. S. Kriz, Introduction to Spectroscopy, 4thEd.,Brooks/Cole Cengage Learning, 2015.
3. R.S. Drago, Physical Methods in Chemistry, Saunders, Thomson Learning, 1977.
4. R.M Silverstein, F. X. Webster, D. J. Kiemle, D. L. Bryce, Spectrometric Identifications of Organic Compounds, 8th Edition, Wiley India Pvt. Ltd, 2015.
5. W. Kemp, Organic Spectroscopy, 3rd Edition, Palgrave Macmillan, 2011.
6. L. D. Field, S. Sternhell, J. R. Kalman, Organic Structures from Spectra, 5th Edition, John Wiley & Sons 2013
7. D.W.H. Rankin, N. Mitzel, C. Morrison, Structural Methods in Molecular Inorganic Chemistry, Wiley, 2013.

Semester II
CH205: Green Chemistry
Credits: 2 (30 h)

Course objective: Introduction to Green Chemistry and its importance in modern chemical laboratory/industry. It is aimed at educating students about the principles and practice of Green Chemistry, and its applicability.

Learning outcome: Students will be able to describe/compare relationships between Green Chemistry and chemical laboratory and industry, particularly in the design of safer chemicals and processes.

1. The Essentials of Green Chemistry: Introduction to Interdisciplinary Study of Green Chemistry, Definition of Green Chemistry **(4 h)**
2. Applying the 12 Principles of Green Chemistry; Green Chemistry Metrics **(5 h)**
3. Waste: production, problems and prevention **(3 h)**
4. Catalysis and green chemistry; Green Chemistry and Sustainability; Green Chemistry to Health and Environment: Inherent Hazards, Challenges; Water oxidation; Conversion of CO_2, Utilising CO_2 as reactant. **(4 h)**
5. Feedstock chemicals, Chemicals from Biomass, Concept of 'platform molecules': Conversion of biomass to value-added products. **(4 h)**
6. Adverse Effects of Chemicals on Health and the Environment; Green Chemistry Problems. **(3 h)**
7. Real World Solutions: Designing for Materials and Energy Efficiency; Designing for Degradation. **(4 h)**
8. Introduction to Sustainability; Aspects of Sustainability Ethics; Designing Sustainable Solutions. **(3 h)**

Books Recommended

1. M. Lancaster, Green Chemistry : An Introductory Text, RSC, 2002
2. P.T. Anastas, J. C. Warner, Green Chemistry : Theory and Practice, Oxford University Press 2008
3. J. H. Clark, F. Deswarte, Introduction to Chemicals from Biomass, 2nd Edition, Wiley 2015

Semester II
CH206: Practical Inorganic Chemistry
Credits: 7

Course objective: Students will be exposed to various experimental skills of qualitative and quantitative analysis and synthetic methods with selected examples. Common spectroscopic techniques like UV-visible, infrared, fluorescence, NMR etc. and non-spectroscopic techniques like PXRD, magnetic susceptibility measurements, electrical conductivity measurements, microscopy, TGA, GC etc. are to be introduced to the students.

Learning outcome: Students will be able to demonstrate experimental skills encompassing synthesis, characterization of different inorganic materials, set-up experiments and use analytical equipments.

1. Qualitative analysis (tertiary mixture, alloy, ore) (semi-micro technique to be preferred)
2. Quantitative analysis (binary mixture, alloy, ore) - Ca-Mg ore, Cu-Zn alloy, Pb-Sn alloy, Ni in an alloy etc.
3. Solution phase synthesis of coordination compounds e.g. vanadylacetylacetonate, potassium trisoxalatometal(III) trihydrate etc.; characterization, properties and applications (e.g. catalysis).
4. Synthesis of coordination compounds through ligand synthesis and spectroscopic characterization, e.g. preparation of bis(*N*,*N*-disalicylideneethylenediammine)(μ-aquadicobalt(II).
5. Solid phase synthesis of coordination compounds (e.g. Reinecke salt, *trans*-bisglycinatocopper(II)) and their properties.
6. Isomerism in coordination compounds. e.g. conversion of chloropentammine cobalt(III) chloride to nitro and nitroso isomers, *cis*- and *trans*-dichlorobis(ethylenediamine)cobalt(III) chloride etc.
7. Preparation of metal(II) isonicotinatetetrahydrates, characterization, use as precursors to metal oxides.
8. Synthesis of metal nanoparticles (Cu, Ag, Au, etc.), characterization and investigation of their optical properties.
9. Synthesis and characterization of semiconductor nanocrystals (CdS, ZnS, ZnO etc.).
10. Preparation of polyoxometallates (e.g. tetrabutylammoniumhexamolybdate(VI)), characterization.
11. Quantitative determination of components in food (Fe, Zn, I, Ca, etc.)
12. Introduction to computational chemistry of simple molecules.

Books Recommended

1. J. Mendham, R. C. Denney, J. D. Barnes, M. Thomas, B. Sivasankar, Vogel’s Textbook of Quantitative Chemical Analysis, 6th Edition, Pearson, 2009.
2. G. Svehla, S. Mittal, Vogel's Qualitative Inorganic Analysis,Pearson Education, 7th Edition. 2013.

Semester III
CH301: Biochemistry
Credits: 3 (45 h)

Course objective: This course will expose the learner to different biochemical systems involved in the process of life.

Learning outcome: Students will be able to describe and interpret the chemical and physical processes of living organisms.

1. **Introduction** (**5 h**)
    - Prokaryotic and eukaryotic cells; structure of plant and animal cells; intracellular organelles and their functions; metabolic processes- catabolism and anabolism; Constituents of cell nucleus, structure of chromosomes, cell division- mitosis and meiosis; composition and functions biological membranes- lipids and lipoproteins.

2. **Biophysical chemistry**: (**10 h)**
    - Bioenergetics- standard free energy change in biochemical reactions, ATP hydrolysis, synthesis of ATP from ADP; biological redox reactions, electron transfer and redox potentials of biologically important half reactions, oxidative phosphorylation.
    - Thermodynamics of biopolymer solutions, osmotic pressure; active transport of ions through cell membrane; muscle contraction; energy generation in living systems; transmission of nerve impulses.

3. **Bioorganic chemistry**: (**20 h)**
    - Nucleic acid chemistry- structure and functions of DNA and RNA, the double helical structure of DNA; unusual DNA structure- DNA hairpins, triple helix, G-quadruplex; stability of the double helix- thermal denaturation and renaturation of DNA double helix; chemical and enzymatic hydrolysis of nucleic acids; DNA replication, RNA transcription and translation of genetic information; chemical basis of heredity.
    - Carbohydrate metabolism- glycolysis, gluconeogenesis and Kreb's cycle.
    - Biochemistry of lipids- biosynthesis of fatty acids, triglycerols, phospholipids, cholesterol and related steroids; prostaglandins.
    - Protein biochemistry- amino acids, biosynthesis of amino acids, activation of amino acids, mechanism of translation, sequencing of amino acids in polypeptides; protein structure- primary, secondary tertiary and quaternary structure of proteins, post-translational modifications and protein folding.
    - Enzymes- classification and catalytic behavior, enzyme kinetics, mechanism of action, factors affecting enzyme activity, enzyme regulators and inhibitors, enzyme models- host-guest chemistry, biotechnological applications of enzymes.

4. **Bioinorganic chemistry**: (**10 h**)
    - Role of metal ions in biology and their toxic effects; Iron management in biological systems – siderophores, ferritin and transferrin; Dioxygen storage and transport – structure of myoglobin and haemoglobin, cooperativity of O_2 binding in haemoglobin, Bohr effect and Hill coefficients; Electron transfer proteins (structure and function) - Fe-S proteins, cytocchromes and plastocyanines; Structure of nitrogenase and its role in di-nitrogen fixation; Structure and function of vitamin B_{12} and mechanism of 1,2-shift reaction; Inorganic therapeutics - chelate therapy, metal based drugs.

Books Recommended

1. D. L. Nelson, M. M. Cox, Lehninger Principles of Biochemistry; 5th edition, 2008 (W. H. Freeman &Co.).
2. R. H. Abeles, P. A. Frey, W. P. Jencks, Biochemistry, Jones and Bartlett Publishers, Boston, 1992.
3. D. Voet, J. G. Voet, C. W. Pratt, Fundamentals of Biochemistry: Life at the Molecular Level, 4th Edition, 2012.
4. I. Bertini, H. B. Gray, S. J. Lippard, J. S.Valentine, Bioinorganic Chemistry; Viva books Pvt. Ltd. 1998.
5. J. A. Cowan, Inorganic Biochemistry: An introduction, 2nd Edition, Wiley, 1997.

Semester III
CH302: Modern Methods of Analysis
Credits: 3 (45 h)

Course Objective: Students will be introduced to modern analytical and non-spectroscopic techniques including thermal methods, diffraction and separation techniques. Analytical techniques like AAS and OES are emphasized upon.

Learning outcome: Students will be able to explain/demonstrate the application of different analytical techniques in chemistry.

1. **Characterization of inorganic molecules: (6h)**
   - Applications of IR, Raman, NMR, EPR, Mössbauer, UV-visible, NQR, MS, electron spectroscopy and microscopy in the determination of structure and physical properties of inorganic compounds

2. **Characterization of organic molecules: (6h)**
   - Applications of IR, UV-visible, NMR, Mass spectrometry, LC-MS in the structure determination of organic compounds.

3. **Microscopy: (8 h)**
   - Development of Microscopy, Optical microscopy, Reflectance, Transmittance, Fluorescence Microscopy, CLSM, Ultra-high resolution microscopy
   - *Electron Microscopy:* Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM): Technique, instrumentation, and applications
   - EDX, SAED
   - Scanning Probe Microscopy (SPM): AFM, STM: Techniques, instrumentation and applications

4. **Thermal Methods: (5 h)**
   - TGA, DTA, DTG, DSC: Techniques, Instrumentation, Applications

5. **Diffraction Techniques: (8 h)**
   - *Powder XRD*: Technique, Instrumentation, Applications
   - *Single Crystal XRD*: Technique, Instrumentation, Applications

6. **Separation Techniques: (5h)**
   - GC, HPLC, GPC: Techniques, Instrumentation, Applications

7. **Analytical Spectroscopic Methods (7 h)**
   - Atomic Absorption Spectroscopy (AAS) – theory, instrumentation and sampling.
   - Atomic (or Optical) Emission Spectroscopy A/OES –theory, instrumentation and sampling, Applications of AAS & A/OES.
   - Electro-analytical methods-polarography, cyclic voltammetry and ion selective electrodes

Books Recommended:

1. D. B. Murphy, M. W. Davidson, Fundamentals of Light Microscopy and Electronic Imaging, Wiley, 2013.
2. D. B. Williams, C. B. Carter, Transmission Electron Microscopy A Textbook for Materials Science, Springer, 2009.
3. P. Eaton, P. West, Atomic Force Microscopy, Oxford University Press, 2010.
4. B. D. Cullity, Elements of X-Ray Diffraction, 3^{rd}Edition, Addison Wesley Publishing Company, Inc., 2004.
5. J. Mendham, R. C. Denney, J. D. Barnes, M. Thomas, B. Sivasankar, Vogel's Textbook of Quantitative Chemical Analysis,6th Edition, Pearson, 2009.
6. A. R. West, Solid State Chemistry and Application, Wiley Student Edition, 1998.

Semester III
CH303: Foundations of Organic Synthesis
Credits: 3 (45 h)

Course objective: Students will be introduced to the basics of retrosynthesis/importance of synthetic planning in organic synthesis.

Learning outcome: Students will be able to identify/explain the concept of selectivity in organic reactions, and describe the stages of synthetic planning in the synthesis of complex molecules.

1. Dynamic stereochemistry (10h)

- Stereospecific and Stereoselective synthesis; classification of stereoselective synthesis, diastereoselective, enantioselective and double stereo-differentiating reactions, nucleophilic addition to aldehyde and acyclic ketones– Cram, Felkin and Felkin-Anh model, Prelog's rule, Stereoselective nucleophilic addition to cyclic ketones (Cram and Felkin-Anh models). Acyclic stereoselection: reactions at α-and β-positions of a chiral center.

2. Carbon-carbon bond formation

- Formation of carbon-carbon single bonds involving Csp3, Csp2 and Csp carbon centers (with emphasis on important name reactions); Carbon-carbon bond forming reactions through enolates (including boron enolates), enamines and silyl enol ethers. Michael addition reaction.
- Formation of C-C multiple bonds involving Csp2 and Csp carbon centers (with emphasis on important name reactions).

3. Retrosynthetic Analysis (12 h)

- Basic principles and terminology of retrosynthesis, synthesis of aromatic compounds, one group and two group C-X disconnections,
- One group C-C and two group C-C disconnections, amine and alkene synthesis, important strategies of retrosynthesis, functional group transposition, important functional group interconversions.

4. Protecting Groups (6 h)

- Protection and deprotection of hydroxy, carboxyl, carbonyl, carboxy amino groups and carbon-carbon multiple bonds; chemo- and regioselective protection and deprotection
- Illustration of protection and deprotection in peptide and carbohydrate synthesis.

5. Introduction to heterocycles

- Structure and reactivity of heterocycles containing one heteroatom (O, N, S) including furan, pyrrole, thiophene, pyridine (Hantzsch pyridine synthesis, Hofmann-Loffler-Freytag reaction), indole (Fischer Synthesis, Bischler Synthesis), quinoline and isoquinoline (Conrad-Limpach reaction, Bischler-Napieralski reaction, Combes reaction, Pictet-Gams synthesis, Skraup/Doebner-von Miller reaction)

Books Recommended:

1. E.L. Eliel, S. H. Wilen, Stereochemistry of Organic Compounds, Wiley, 2010
2. F. A. Cary, R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5thEdition, Springer, 2009.
3. M. B. Smith, Organic Synthesis, 2ndEdition, McGraw Hill Higher Education, 2005.
4. W. Carruthers , I. Coldham, Modern methods of Organic Synthesis, Cambridge University Press, 2005.
5. J. J. Li, Name Reactions in Heterocyclic Chemistry, Wiley, 2006
6. R. O.C. Norman, J. M. Coxon, Principles of Organic Synthesis, 3rd Edition, CRC Press

Semester III
CH304: Seminar Course
Credit 2 (30 h)

Course objective: This is a core course, where students will be prepared for scientific presentation and literature survey to help convey scientific information in organized and comprehensive way. Students will be required to present a seminar on identified topic at the end of the semester for successful completion of this course.

Learning outcome: On successful completion of this course students will acquire better communication and presentation skills.

Semester III
CH305: Practical Physical Chemistry
Credits: 7

Course objective: This is a core laboratory course introducing some experimental and theoretical experiments of physical chemistry. The objective of the course is to introduce two types of experiments. The first is involved with basic physical chemistry such as chemical kinetics, theoretical chemistry, thermodynamics, photochemistry etc. The objective of second type of experiments is to introduce students to some modern techniques of analysis such as spectrophotometry, electrochemical analysis and surface chemistry.

Learning outcome: From this course, the students will understand physical chemistry from experimental point of view. Moreover, they will learn some modern methods of analysis required in different area of research.

Unit 1: [Minimum 10 experiments, at least 3 experiments from each section, i, ii, iii]

(a) Experiments on Chemical Kinetics

1. Determination of the temperature coefficient and energy of activation of acid hydrolysis of methyl acetate, using least squares calculation.
2. Study of the kinetics of reaction between iodine and acetone in acidic medium by half-life period method and determination of the order with respect to iodine and acetone.
3. Study of the saponification of ethyl acetate by sodium hydroxide and determination of the order of the reaction and energy of activation.
4. Study of the autocatalytic reaction between oxalic acid and $KMnO_4$ and determination of the order of the reaction.
5. Study of the decomposition kinetics of the formation of complex between sodium sulphide and sodium nitroprussidespectrophotometrically. Determination of the rate constant and order of the reaction.
6. Study of the kinetics of the reaction between peroxydisulphate and potassium iodide and to find the influence of ionic strength on the rate constant.
7. Study of the kinetics of oxidation of ethanol by chromium(VI) and to find the rate constant of the reaction. Also find the order of the reaction by half-life period method.
8. Study of the double exponential time dependence of the reduction of Cr(VI) by glutathione in an aqueous medium and to obtain the rate constants of the process. (EPC , Halpern Ex. No. 23, 381)
9. Determination of the rate constants for the α-chymotrypsin-catalyzed hydrolysis of an ester. (EPC , Halpern Ex. No. 24, 395)
10. Determination of the mechanism and rate constant for the oxidation of magnesium by hydrochloric acid. ((EPC, Halpern Ex. No. 26, 425)
11. Determination of the relative strength of two acids (HCl and H_2SO_4) by studying the hydrolysis of an ester (methyl acetate/ ethyl acetate). [Yadav, 288]
12. Investigation of the inversion of cane sugar in presence of HCl and H_2SO_4 and hence determination of the relative strengths of the two acids.
13. Investigation of the inversion of cane sugar in presence of acid and hence determination of the activation energy of the reaction.

(b) Experiments on Conductometric Titrations

1. Determination of the equivalent conductivity of acetic acid at infinite dilution by Kohlrausch's method and hence to find the degree of dissociation constant of the acid.
2. Comparison of the relative strength of acetic acid and monochloroacetic acid by conductance measurement.
3. Determination of the degree of hydrolysis and hydrolysis constant of aniline hydrochloride /sodium acetate.
4. Determination of the strength of the components of the following binary mixture by conductometric titration.
   (a) Hydrochloric acid and acetic acid
   (b) Sulphuric acid and copper sulphate
   (c) Hydrochloric acid and potassium chloride
   (d) nitric acid and sulphuric acid
5. Determination of the amount of each component of the following ternary mixture by conductometric titration.
   Hydrochloric acid, acetic acid and copper sulphate
6. Determination of the degree of hydrolysis and hydrolysis constant of CH_3COONa of NH_4Cl by conductance measurement.
7. Determination of the concentration of $AgNO_3$ by conductometric titration against KCl solution.

(c) Experiments of Spectrophotometry etc.

1. Verify Beers law and determine concentration of
   (a) $K_2Cr_2O_7$ (b) Organic dyes like methylene blue, Rhodamine B (c) $CuSO_4$
2. Determination of the concentration of chromium and manganese in a mixture of dichromate and permanganate by spectrophotometric method.
3. Determination of the composition of iron salicylic acid complex spectrophotometrically by Job's method of continuous variation.
4. Investigation of the complex ion formation between Ni^{2+} and o-phenanthroline by Job's method.
5. Determination of the refractive index of liquid like carbon tetrachloride and to find the radius of its molecule.
6. Verify the mixture law of refraction and draw the calibration curve for mixtures like glycerol water, n-heptane/ n-hexane. Hence determination of the composition of an unknown mixture of two components.
7. Investigation of the reaction between acetone and iodine by colorimetry.
8. Determination of the refractive index of a given liquid by Abbe refractometer and to find the molar and specific refractions.

Unit 2: [Minimum 5 experiments, at least 1 experiments from each section, i, ii, iii]

(i) Experiments on pH metric Titrations

1. Determination of the dissociation constant of oxalic acid by using Hendersen's equation.
2. Determination of the dissociation constant of acetic acid by using Hendersen's equation
3. Finding the amount of the components of the following mixtures using pH metric titration
   (a) Hydrochloric acid + Acetic acid
4. Finding the amount of the components of the following mixtures using pH metric titration
   (a) Hydrochloric acid + Oxalic acid
5. Determination of the pH of a buffer solution by using quinhydrone electrode.
6. Potentiometric estimation of strength of solutions of hydrochloric acid and acetic acid individually and a mixture of the two using standard sodium hydroxide solution.
7. Titration of ferrous ammonium sulphate against potassium dichromate potentiometrically and determination of the standard electrode potential of the ferrous/ferric system.

(ii) Electrochemical experiments: Cyclic voltammetry

1. Cyclic voltammetry of a standard solution at different scan rates and calculation of redox potential ofelectro-active species.
2. Determination of diffusion coefficient from cyclic voltammetry
3. Determination of Electrode surface area from Cyclic voltammetry
4. Determination of rate of heterogeneous electron transfer from cyclic voltammetry
5. Chronocoulometry of a redox dye and determination of amount adsorbed on to the electrode surface
6. Electrochemical impedance spectra of redox molecules and determination of charge transfer resistance.

(iii) Adsorptio-desorption on porous materials, Equilibrium study, kinetic study, thermodynamic studies

1. Adsorption of dye on activated carbon and analysis of result by different adsorption models.
2. Determination of adsorption kinetics of dye on activated carbon.
3. Determination of desorption kinetics of dyes from adsorbents
4. Determination of thermodynamic quantities ΔH, ΔS and ΔG of dye adsorption on activated carbon.

Unit 3: [Minimum 5 experiments, at least 1 experiments from each section, i, ii]

(i) Experiments of Theoretical Chemistry

1. Least squares fitting and plotting linear and exponential graphs using computer.
2. Potential energy diagram of hydrogen molecule ion with the help of fortran programming.

(ii) Miscellaneous Experiments

1. Determination the molar mass of a polymer by viscometric method.
2. Study of the variation of surface tension of a solution of n-propyl alcohol/ethanol with concentration and determination of the limiting cross-sectional area of the alcohol molecule.

3. Determination of the partial molar volume of methanol/ethanol/formic acid by graphical method by determining the densities of solutions at different concentrations.
4. Determination of the influence of NaCl, naphthalene and succinic acid on the critical solution temperature of phenol-water system using 0.5, 1 and 1.5 % concentrations.
5. Study of the complex formation between Cu^{2+} ion and ammonia by distribution method and to find the composition of the complex.
6. To measure the viscosity of glycerol and its temperature dependence using the falling sphere method. (ref. Halpern, Expt. 18, Pg-307).
7. Determination of the molecular surface energy and the association factor for ethyl alcohol. (Ref. Yadav Pg. 88)
8. Determination of the heat capacity of a calorimeter and hence determination of the enthalpy of solution of NH_4Cl.
9. Determination of the Van't Hoff factor for an electrolyte by cryoscopic method.
10. Determination of the percentage composition of binary mixture of non-electrolyte (urea and glucose) by cryoscopic method.
11. Study of the variation of solubility of $Ca(OH)_2$ in NaOH solution and hence to determine its solubility product.
12. Determination of the CMC of a detergent by surface tension measurement.
13. Determination of the equilibrium constant of the reaction:$KI + I_2 \leftrightharpoons KI_3$ by distribution method.
14. Determination of the formula of the complex formed between Cu^{2+} and NH_3 by distribution method.
15. Determination of the heat capacity of a calorimeter and hence determination of the enthalpy of solution of NH_4Cl.

Books Recommended

1. J. B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 27th Edison, 2008.
2. J. N. Gurtu and A. Gurtu, Advanced Physical Chemistry Experiments, PragatiPrakashan, 6th Edition, 2014.
3. M. Halpern, Experimental Physical Chemistry, 2nd Edition, Prentice Hall, Upper Saddle River, NJ 07458
4. Other Sources:*Journal of Chemical Education*, ACS Publications.

Semester III
CH306: Solid State & Materials Chemistry
Credits: 3 (45 h)

Course Objective: Students will be introduces to the interdisciplinary field of solid state and materials chemistry, and the development of materials for various applications.

Learning outcome: Students will be able toexamine/differentiate between different materials, and design/plan novel materials for applications.

1. **Introduction to Materials(8 h)**
   - Classification of Materials: Metals, Ceramics, Polymers, Composites
   - Advanced materials: Smart materials, Carbon nanomaterials, Semiconductor nanomaterials, Materials for the future, LED, OLED, Superconductors.

2. **Solid State Chemistry:**

   - *Synthesis of solids:* (**7 h)**

   High-temperature ceramic methods including precursor based methods and the sol-gel method and modifications thereof; hydrothermal method; chemical vapour deposition method; intercalation method; crystal growth techniques – brief introduction; Fabrication of nanomaterials – top-down and bottom-up approaches; solution-based synthesis of nanoparticles; other methods of nanomaterial synthesis – brief overview.

   - *Theory* :**(8 h)**

   Structure, Band structure, Defects, Phase diagrams, Phase transition, Physics of nanoscale materials, Quantum confinement effect.

   - *Properties:* (**8 h)**

   Chemical, Magnetic, Optical, Mechanical Properties, Thermal, Electrical, Sensors, Energy materials

   - *Characterization techniques:* (**7 h)**

   Routine characterization tools – UV –visible spectroscopy, Fluorescence, NMR, FTIR, TGA/DSC, Particle size analyzer, Zeta potential, Powder X-ray diffraction, Scanning electron microscopy, Transmission electron microscopy, X-ray photoelectron spectroscopy, Atomic force microscopy – Scanning probemicroscopy, Electron beam lithography, Electroanalytical methods.

3. **Organic Solid State Chemistry(4 h)**
   - Organic semiconductors, liquid crystals, energy materials, smart materials

4. **Materials Design(3 h)**
   - Economic, Environmental and Societal issues.

Books Recommended

1. P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong, Shriver & Atkins' Inorganic Chemistry, 5th Ed., OUP 2010.
2. B. Fahlman, Materials Chemistry, 2nd Ed., Springer, 2011
3. L. Smart, E. Moore, Solid State Chemistry: An Introduction, 4thEd. CRC Press 2012.
4. A. R. West, Solid State Chemistry and its Applications, Wiley Student Edition, John Wiley & Sons, 2007.
5. R. Balasubramaniam, Callister's Materials Science and Engineering, 2nd Edition, Wiley, 2014.

Semester III
CH307: X-ray Crystallography
Credits: 3 (45 h)

Course objective: This course is aimed at educating post-graduate students about crystals, crystal symmetry, including the principles and practices of X-ray crystallography. The course shall emphasize on the practical aspects of this technique,and the salient featuresof crystal engineering, material science as well as macromolecular (biological) crystallography.

Learning outcome: Students will be able to explain the basis of structure determination, interpret experimental data, and understand literature related to X-ray crystallography.

1. **The crystalline state (5 h)**
   - Crystallization and crystal growth, symmetry of crystals, space groups, interrelation of lattice symmetry, crystal symmetry and diffraction symmetry, determination of space groupsfrom systematic absences, International Tables of Crystallography

2. **Principles of X-ray diffraction (10 h)**
   - X-ray scattering by a crystal, Structure factors and electron density, Braggs' law, powder and single crystal X-ray diffraction, the phase problem, crystal structure solution, refinement of crystal structure, Small angle X-ray scattering (SAXS)

3. **X-ray Diffraction in practice (15 h)**
   - Generating X-rays – from sealed tubes to synchrotrons, data acquisition equipment – single crystal and powder X-ray diffractometers, Crystallographicsoftwares, solving and refining structures, analysing structures, reporting crystallographic findings in literatureand reports

4. **Applications of X-ray crystallographic methods (15 h)**
   - Applications of the powder X-ray diffraction method - phase identification, thin film and nanomaterial characterization, and other applications
   - Applications of single crystal X-ray diffraction method - molecular and crystal structure determination, supramolecular structural aspects, crystal engineering
   - Macromolecular crystallography-Biological structure determination
   - Structural databases – CSD, ICSD, PDF and PDB- uses in chemistry, physics and biology

Books Recommended

1. Structure Determination by X-ray Crystallography, by R.A. Ladd and M.F.C. Palmer, Springer, 1985.
2. X-ray Structure Determination: A Practical Guide, 2^{nd} Edition by G.H. Stout and L. Jensen, Wiley Interscience, 1989.
3. Fundamentals of Crystallography, 2^{nd} Edition, by C. Giocovazzo et al., Oxford University Press, 2002.

Semester III
CH308: Environmental Chemistry
Credits: 3 (45 h)

Course objective: Students will be introduced tothe concerns/prospective about environment, Kyoto Protocol. Students are expected to understand different aspects of environmental chemistry, chemistry of atmosphere, soil and water.

Learning Outcome: Students will be able to demonstrate an understanding of environmental chemistry, viz. air, water and soil chemistry and identify the relationships between atmosphere, solar radiation and ozone formation.

1. **Environmental Chemistry: An Introduction (5 h)**
   - Environment & environmental chemistry, importance of the study. Environmental composition, chemical processes, anthropogenic effect and environmental pollution. Environment - global concern and prospective, Kyoto Protocol.

2. **Chemistry of the atmosphere (16 h)**
   - Atmosphere & atmospheric chemistry, importance of the atmosphere, solar influence on the chemical composition of atmosphere, photochemical and chemical reactions in atmosphere, ions and radicals in the atmosphere.
   - Solar radiation and plant and animal life, stratospheric ozone, ozone formation reactions, ozone destruction reactions, Montreal Protocol, antarctic and arctic ozone hole.
   - Inorganic air pollutants, control of particulate emissions, carbon oxides & global warming, sulpher dioxide &sulpher cycle, nitrogen oxides in atmosphere, acid rains.
   - Organic air pollutants: examples, smog, types of smog, photochemical smog, smog forming reactions of organic compounds mechanism of smog formation effects of smog.

3. **Soil Environmental Chemistry (12 h)**
   - Soil and soil formation- physical weathering and chemical weathering, soil organic matter, chemical properties of soil-cation exchange cap., pH, macro and micronutrients, leachate formation, Environmental issues associated with soils-nutrient leaching, acidification, salinity and alkalinity, metal contamination.

4. **Environmental Chemistry of Water (12 h)**
   - Distribution of chemical species in water, phosphorus and sulphursystems , acidity and alkalinity, chelation in water, humic matter in water-origin, formation and environmental role.
   - Partitioning of small organic molecules between water and soil or sediment, octanol – water partition coefficient.
   - Water pollution, inorganic pollutants, organic pollutants, eutrophication, radio-nuclides in aquatic environment.

Books Recommended

1. S.E. Manahan, Fundamentals of Environmental Chemistry, Lewis Publishers
2. G. W. Vanloon, S. J. Duffy, Environmental Chemistry, 3rd Edison, Oxford University Press

Semester III
CH309: Surface Chemistry and Catalysis
Credits: 3 (45 h)

Course objective: This is a core interdisciplinary course. It covers basic surface chemistry and applications of surface chemistry mainly on catalysis. Modern experimental techniques such as photoelectron spectroscopy, Auger electron spectroscopy, high resolution energy loss spectroscopy etc. will be introduced in this course. This course will also cover homogenous catalysis.

Learning outcome: This course will help the students to understand an important subject "surface chemistry" from the interdisciplinary point of view. Surface chemistry has many industrial applications including catalysis. The students will learn from the basic physics and chemistry to applications of material surfaces through this course.

1. The solid-liquid interface (8 h)

- Surface energy from solubility changes, surface energy from immersion, contact angle, contact angle hysteresis, experimental methods and measurement of contact angle, theories of contact angle phenomena, adsorption of non-electrolytes from dilute solutions, irreversible adsorption, adsorption in binary liquid systems, adsorption of electrolytes.

2. The solid-gas interface (8 h)

- Surface area of solids, structure and chemical nature of solid surfaces, nature of the solid adsorbate complex, adsorption of gases and vapours on solids,Langmuir adsorption isotherm, the BET and related isotherms, isotherms based on equation of state of the adsorbed films, potential theory, phase transformations in the multiplayer region, thermodynamics of adsorption, critical comparison of various models for adsorption.

3. Physisorption and Chemisorption 3 (12 h)

- Physical adsorption on heterogeneous surfaces, rate of adsorption, adsorption on porous solids: hysteresis
- Chemisorption and catalysis, chemisorption isotherms, kinetics of chemisorption, surface mobility, chemisorption bond, heterogeneous catalysis, transition state theory, specificity and selectivity in catalysis, catalytic activity and strength of chemisorption, Langmuir-Hinshelwood and Eley-Rideal mechanism, electronic factors in catalysis by metals, geometric factors in heterogeneous catalysis, Photo-catalytic reactions by metal oxides.

4. Surface Characterization Techniques (10 h)

- Ultra high vacuum for surface studies, Low energy electron diffraction, Photoelectron spectroscopy, Inverse photoemission spectroscopy, Scanning probe microscopy, Auger electron spectroscopy, Infrared spectroscopy, High resolution electron energy loss spectroscopy, Low energy ion scattering spectroscopy.

5. Homogenous Catalysis (7 h)

- Atom transfer and electron transfer processes, role of transition metal ions with spectral reference to Cu, Pd, Pt, Co, Ru, and Rh, catalysis in non-aqueous media, rate of homogenous catalytic reactions, turnover number and frequency, catalysis of isomerization, hydrogenation, oxidation and polymerization reactions, asymmetric catalysis, biocatalysis, photo-activated catalysis and metal clusters in catalysis, phase transfer catalysis.

Books Recommended

1. A.W. Adamson, A.P. Gast, Physical Chemistry of Surfaces, John Wiley and Sons, Canada, 1997.
2. R.H. P. Gasser, "An introduction to chemisorption and catalysis by metals", Oxford, 1985.
3. A. Clark, "Theory of adsorption and catalysis", Academic Press, New York, 1970.
4. D.K. Chakrabarty, "Adsorption and catalysis by solids", Wiley Eastern Ltd. 1990.
5. J.M. Thomas, W.J. Thomas, "Introduction to principles of heterogeneous catalysis", Academic Press, New York, 1967.
6. G. A. Somorjai, "Introduction to surface chemistry and catalysis", 2nd Edition Wiley-Blackwell, 2010.

Semester III
CH310: Food Chemistry
Credits: 3 (45 h)

Course objective: Students will be introduced to the importance of food/nutrition, function of foods and prevention of deficiencies. Aspects related to various classes naturally occurring chemical species/additives, their isolation, characterization and synthesis will be discussed

Learning outcome: Students will be able to explain/compare food asmajor dietary constituents,naturally occurring food, their energy/nutritional values.

Learning objective:

1. **Basic concepts of food & nutrients** **(2 h)**
   - Understanding the relationship between food, nutrition & health
   - Functions of food—Physiological & Social

2. **Major dietary constituents & energy needs** **(12 h)**
   - Functions, dietary sources and clinical manifestationsof deficiency/excess of the following nutrients:
     (i) Proteins and Amino Acids
     (ii) Carbohydrates
     (iii) Lipids, Sterols & metabolites
     (iv) Minerals
     (v) Vitamins : Fat soluble vitamins (A, D, E, K)
     Water Soluble Vitamins (Thiamine, Riboflavin, Niacin,
     Biotin, Pyridoxine, Cyanocobalamin)
     (vi) Other imp. Compounds of nutritional relevance (Cholin, Cysteine,Carotenoids)

3. **Food groups** **(7 h)**
   Selection, nutritional contribution and changes during Cooking/Ripening/storage of the following groups:
   - Cereals
   - Pulses
   - Fruits and vegetables
   - Milk and milk products
   - Eggs, Meat, Poultry & fish
   - Fats & oils

4. **Nutritional needs during life cycle** **(6 h)**
   - Body composition, Influence of Nutrition, Physical Activity, Growth and Aging
   - Maternal Nutrition, Nutritional Requirement during Infancy, Childhood
   - Diet, Nutrition and Adolescence
   - Nutrition in the Elderly

5. **Prevention and management of deficiencies** **(6 h)**
   Causes, Symptoms, Treatments, Prevention of the following
   - Protein-Energy Malnutrition(PEM) amongst Children
   - Vitamin A-Deficiency (VAD)
   - Iron Deficiency Anemia (IDA)
   - Fluorosis
     - Over nutrition: Obesity, Coronary Heart Disease, Diabetes (Type I & II)
   - Diet, Nutrition & Cancer

6. **Dietary goals & guidelines** **(10 h)**
   - National Perspectives
   - Nutritional Perspectives of Vegetarian Diets
   - Social Health Issues – Smoking, Alcoholism, Drug Addiction, AIDS and AIDS Control Programs
   - Food Preservation & Food Additives &Colourants

7. **Entrepreneurship Development** **(2 h)**
   - Scope of Food based items for Entrepreneur Development in North East India & Identification of Resources
   - Development of a Project Plan

Books Recommended

1. S. R. Mudambi, M. V. Rajagopal, Fundamentals of Foods, Nutrition and Diet Therapy, 5th Ed, New Age International, 2012
2. B.Srilakshmi, Nutrition Science, New Age International, 2012.
3. Handbook of Food and Nutrition, 5th Edition, BAPPCO, 1986.

4. G. M. Wardlaw, J. S. Hanpl, Perspectives of Nutrition, McGraw Hill, 2007.
5. S. Sari, A. Malhotra, Food Science, Nutrition and Food Safety, Pearson India Ltd, 2014.
6. C. Gopalan, B. V. Rama Sastri, S. C. Balasubramanian, Nutritive Value of Indian Foods, NIN, ICMR, 2011.
7. M. S. Bamji et al., Textbook of Human Nutrition, Oxford & IBH Pub Co Pvt Ltd, 2009.
8. P. Lakra, M. D. Singh, Text book of Nutrition & Health, 1st Edition, Academic Excellence, 2008.
9. WHO Child Growth Standards, World Health Organization, Geneva
10. William's Nutrition & Diet Therapy, Stacy Nix, 13thed, 2009, Elsevier-Mosby
11. Guidelines for Indians – A Manual. National Institute of Nutrition, ICMR, Hyderabad
12. M. E. Shils et al., Modern Nutrition in Health and Disease, 9th Edition, Lippincott Williams & Wilkins, 1998.
13. J. B. Knight, L. H. Kotschevar, Quantity Food Production Planning &Management, 3rd Edition, John Wiley & Sons, 2000.

Semester IV
CH401: Natural Products Chemistry
Credits: 4 (60 h)

Course objective: All over the world chemists are turning to the nature for finding new materials which make the study of natural products a very important subject. The objective of the course is to teach several classes of natural products, their isolation, synthesis, biosynthesis etc.

Learning outcome: On completion, students will be able to identify different types of natural products. Students will be able to describe important methods of extraction, their synthesis, and biosynthesis.

1. **Introduction (5 h)**
   - Natural products chemistry: a general treatment. Primary and secondary metabolites.

2. **Carbohydrates (15 h)**
   - Open chain and ring structure of monosaccharides,
   - Reactions of the anomericcentre, Reactions of hydroxyl groups, Cyclic acetals, Glycosyl activation
   - Chemical disaccharide formation, Enzymatic dissacharide formation, Introductory chemical glycobiology

3. **Terpenoids(15 h)**
   - Introduction to terpenoids, isoprene and biogenetic isoprene rule,
   - Biosynthesis of mono and sesquiterpenoids, discussion on caryophylene, longifolene, santonin, abietic acid, and taxol.

4. **Steroids(9 h)**
   - Introduction to steroids: cholesterol, bile acids, sex hormones, cardiac glycosides and corticosteroids.

5. **Alkaloids (8 h)**
   - Introduction to alkaloids, physiological activity of alkaloids, Discussion on morphine, and reserpine.

6. **Carotenoids(8 h)**
   - General Introduction, Discussion on alpha-, beta- and gamma-carotenes, vitamin-A.

Books Recommended:

1. S. V. Bhat, B.A. Nagasampagi, M. Sivakumar, Chemistry of natural products, Springer Narosa, 2005.
2. P. S. Kalsi, S. Jagtap, Pharmaceutical, medicinal and natural products chemistry, Alpha Science International Ltd. 2013.
3. N. R. Krishnaswami Chemistry of natural products-A Unified Approach, University Press, 1999.
4. I. L. Finar, Organic Chemistry, vol-2, Pearson, 2009.
5. B. G. Davis, A. J. Fairbanks, Carbohydrate Chemistry, Oxford University Press, 2002.
6. S. K.Talapatra, B. Talapatra, Chemistry of Plant Natural Products, Springer, 2015.
7. C. Sell, A Fragrant Introduction to Terpenoid Chemistry, RSC, 2003.

Semester IV
CH402: Advanced Organic Synthesis
Credits: 4 (60h)

Course objective: This course is aimed at educating students about the principles of organic synthesis, and the concepts of planning a multistep synthesis (‘Retrosynthesis’). This course will also provide a glimpse of recent trends and developments in organic synthesis.

Learning outcome: Students will be able to design synthesis strategies, and describe important methods for synthesizing complex molecules.

Unit 1: Synthetic methods –I (15h)

- Formation of carbon-carbon single bonds involving Csp3, Csp2 and Csp carbon centers (with emphasis on important name reactions); Carbon-carbon bond forming reactions through enolates (including boron enolates), enamines and silylenol ethers. Michael addition reaction.
- Formation of C-C multiple bonds involving Csp2 and Csp carbon centers (with emphasis on important name reactions).

Unit 2: Synthetic methods –II (10h)

- Formation of carbon-heteroatom bonds: New methods for the construction of C-N, C-O, C-S and C-X bonds (including aspects related to the activation of C-H bonds)

Unit 3: Asymmetric Synthetic Methods (15 h)

- Enantioselective synthesis (alkylation, allylation and crotylation reactions), use of chiral reagent; Chiral catalyst and chiral auxiliary; Use of chiral auxiliaries (Evans oxazolidones, Oppolzersultams, Myers amides, Schöllkopf Chiral Auxiliaries).
- Concepts of asymmetric synthesis: Kinetic resolution (including enzymatic resolution), desymmetrization reactions
- Asymmetric reactions: Epoxidation (Sharpless, Jacobsen, Shi), Dihydroxylation (Sharpless), Reduction (Noyori, Corey, Pfaltz)

Unit 4: Construction of Ring Systems (12 h)

- Different approaches towards the synthesis of three, four, five and six-membered rings; photochemical approaches for the synthesis of four membered rings, oxetanes and cyclobutanes. Diels-Alder reaction (inter- and intra-molecular), ketene cycloaddition (inter- and intramolecular), Pauson-Khand reaction, Bergman cyclization; Nazarov cyclization, cation-olefin cyclization and radical-olefin cyclization,
- Heterocyclic rings (with two or more heteroatoms): Pyrazoles, isoxazoles, thiazoles, triazoles and pyrimidines (Claisen synthesis, Fischer synthesis)
- Inter-conversion of ring systems (contraction and expansion); construction of macrocyclic rings, ring closing metathesis.

Unit 5 Synthesis of Complex Molecules (8 h)

- Total synthesis of Terpenes(caryophylene) and alkaloids (e.g. Reserpine, morphine).

Books Recommended:

1. S. Warren, Organic Synthesis:The Disconnection Approach, Wiley India Pvt. Ltd. 2004.
2. F. A. Cary, R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edition, Springer, 2009.
3. M. B. Smith, Organic Synthesis, 2ndEdition,McGraw Hill Higher Education, 2005.
4. W. Carruthers , I. Coldham, Modern methods of Organic Synthesis, 1st South Asian Edition Cambridge University Press, 2005.

Semester IV
CH403: Quantum and Computational Chemistry
Credits: 4 (60h)

Course objective: Students will be able to understand of advanced theories and techniques of quantum mechanics, modern ab-initio approaches to electronic structure calculation and properties of molecules.

Learning outcome: Students will be able to explain/compare and analyse the quantum mechanical (approximate) formalisms, and be apply these formulation to setting up of basis set functions for structure calculation and properties of molecules.

1. **Mathematical Review (10h)**
   - Linear algebra, Three dimensional vector algebra, Matrices, Determinants, N-dimensional complex vector spaces , Change of basis, The eigen value problem, Functions of matrices
2. **Formulation of quantum mechanics (15h)**
   - Schrodinger's and Heisenberg's formulation of quantum mechanics
   - The time dependent Schrodinger equation, Separation of Variables and Reconstitution of the Wavepacket, Expectation Values, The Free-Particle Wave packet, General Solution, The Center of the Wavepacket, The Dispersion of the Wavepacket, The Gaussian Wave packet, The Gaussian Free Particle, General Properties of Gaussian Wavepackets
3. **Many electron wave functions and operators (15h)**
   - Many Electron Wave Functions and Operators, The Electronic Problem, Atomic Units
   - The Born-Oppenheimer Approximation, The Antisymmetry or Pauli Exclusion Principle, Orbitals, Slater Determinants, and Basis Functions, Spin Orbitals and Spatial Orbitals, Hartree Products, Minimal Basis H_2 Matrix Elements, Notations for One- and Two-Electron Integrals, Coulomb and Exchange Integrals.
4. **Hartree-Fock approximation(20h)**
   - The Hartree-Fock Approximation, The Minimal Basis H_2 Model, Excited Determinants, Form of the Exact Wave Function and Configuration Interaction,
   - The Fock Operator, The Canonical Hartree- Fock Equations, Interpretation of Solutions to the Hartree-Fock Equations, Orbital Energies and Koopmans' Theorem, The Hartree-Fock Hamiltonian, Closed-Shell Hartree-Fock: Restricted Spin Orbitals, Introduction of a Basis: The Roothaan Equations, The Charge Density, Expression for the Fock Matrix, The SCF Procedure, Polyatomic Basis Sets, Contracted Gaussian Functions, Minimal Basis Sets: STO-3G, Double Zeta Basis Sets: 4-31G, Polarized Basis Sets: 6-31G* and 6-31G**

Books Recommended:

1. A. Szaboo, N. S. Ostlund, Modern Quantum Chemistry, 1st Edition (Revised), 2015.
2. David J. Tannor, Introduction to Quantum Mechanics (A time-dependent perspectives), University Science Books, 2007 .
3. Ira N. Levine, Quantum Chemistry, 7th Edition, PHI Learning Pvt. Ltd., 2014.

Semester IV
CH404: Catalysis Science & Technology
Credits: 4(60h)

Course objective: Students will learn about catalysts, their preparation methods and their use in catalytic reactors (i.e. activation & deactivation of catalysts and their regeneration).

Learning outcomes: Students will be able to identify/explain different types of catalysts, preparation methods, their activation/deactivation including design of catalytic reactors. Students will be able to formulate the design/synthesis new catalysts.

1. **Catalysts synthesis and preparation (15h)**
   - Catalyst preparation methods – precipitation and co-precipitation – sol gel process–Dispersed metal catalysts; support materials; preparation and structure of supports; surface properties – preparation of catalysts – interaction of metal compound with substrate surface – metal distribution within catalyst pellets – metal cluster compounds as active precursors – pre-activation treatment – drying and calcinations – activation process. Bulk catalysts and supports.Heteropoly compounds – Solid superacids.carbon as catalyst support – carbon as catalyst.
   - Catalyst manufacture– scope and goals – catalysts prepared by precipitation – solution and slurry transfer – filtration – drying: calcining; ion exchange; extrusion; crushing and screening to produce granules; coating etc.

2. **Zeolites, mesoporous materials and clays (20h)**
   - Synthesis of aluminosilicate zeolites and related silica based materials – structure, composition, zeolite synthesis, mechanism and chemistry–zeolites obtained from various reaction systems – synthesis of some selected important zeolites – titanosilicates – activation of zeolites. Modification of zeolites – ion exchange – metals supported on zeolites– dealumination and desilication of zeolites; Shape selective catalysis in zeolites.
   - Pillared clays– properties of pillared clays.Use of coordination and organometallic compounds as pillaring.pillaring of acid activated clays
   - Mesoporous materials - ordered mesoporous materials –synthesis of silica molecular sieve materials - characterization of mesoporous molecular sieves – catalytic properties of mesoporous materials
   - Catalytic applications of zeolite, clays and mesoporous materials.

3. **Catalytic reactors, deactivation of catalysts (10h)**
   - Deactivation of catalysts – classification of catalyst deactivation processes; general aspects of catalyst deactivation – poisoning of catalysts, poisoning of metallic catalysts, poisoning of non-metallic catalysts – poisoning of bifunctional catalysts – coke formation on catalysts – metal deposition on catalysts – sintering of catalysts; Regeneration of deactivated catalysts.
   - Design of catalytic reactors. Mass flow and heat flow minimisation.

4. **Energy and catalysis (15h)**
   - Energy related catalysis – Perspectives in oil refining – Steam reforming – Water gas shift– Methanol synthesis – CO and CO_2 hydrogenation – Methanol to hydrocarbons – Hydrotreating reactions – Catalytic reforming – Catalytic cracking, Hydrocracking. Aromatization of light alkanes, Catalytic coal gasification, Catalysis in coal liquefaction; Fuel cells – Heterogeneous photocatalysis
   - Alkylationof aromatics: Isomerization and trans-isomerization – Dehydrogenation reactions – Hydrogenation reactions – Hydroformylation – Selective oxidations. Control of pollution from automobile exhaust-catalytic conveters, abatement of nitrogen oxides and odours.

Books Recommended:

1. G. Ertl, H. Knozinger, J. Weitkamp (Eds), Preparation of Solid Catalysts, WileyVCHVerlag, 1999.
2. J.R. Anderson, M. Boudart (Eds), Catalysis, Science and Technology, Vol 6, Springer-Verlag, 1984.
3. J. Weitkamp and L. Puppe (Eds), Catalysis and zeolites – fundamentals and applications, Springer-Verlag, 1999.
4. A. Gil, L.M. Gandia, M.A. Vincente, Catalysis Reviews Science and Engineering, 42 (2000) 145-212.
5. M. Hartmann, L. Kevan, Chemical Reviews, 99 (1999) 635-663.
6. A.B. Stiles, T.A. Koch, Catalyst manufacture, Marcel Dekker Inc., 1995.
7. R. Hughes, Deactivation of catalysts, Academic press, 1984.
8. G. Ertl, H. Knozinger, J. Weitkamp, Handbook of Heterogeneous Catalysis,Vol 4 and 5, Wiley-VCH, 1997.
9. R. J. Farrauto, C.H. Bartholomew, Fundamentals of Industrial Catalytic Processes, Blackie Academic, Chapman and Hall, 1997.
10. R. Pearce, W.R. Patterson, Catalysis and Chemical processes, Academic press, 1981.
11. J. Weitkamp, L. Puppe (Eds), Catalysis and zeolites – fundamentals and applications, Springer-Verlag, 1999.

Semester IV
CH405: Nanoscience and Nanotechnology
Credits: 4(60h)

Course Objective: Students will be introducedto underlying physical/chemical principles of nanoscience, synthetic strategies, materials characterization and technological impact.

Learning outcome: Students will be able to identify/analyze/characterize different types of nanomaterials,their properties, and various applications.

1. **Introduction to Nano (5 h)**
   - The Science behind Nanotechnology, History of Nanoscience , Definition of Nanometer, Nanomaterial, and Nanotechnology , Classification of Nanomaterial , Nanotechnology from the Perspective of Medieval Period , Nanomaterials in nature.

2. **Concepts of Solid-State Physics Relevant to Low-Dimensional Systems (10 h)**
   - Crystal Symmetries, Crystal Directions, and Crystal Planes , Band Structure, Classification of Solid-State Materials , Bulk Properties of Materials , Magnetic Materials, Effect of Size Reduction on Bulk Properties , Optoelectronic Property of Bulk and Nanostructures , Electronic Structure of Nanomaterial and the Fermi Surface, Luminescence from Nanoparticles, Thermodynamics of Nanomaterial

3. **Quantum Mechanics of Low-Dimensional Systems (10h)**
   - Energy Considerations: Bound States and Density of States, Quantum Confinement, Super lattices, Band Offsets, Quantum Transport in Nano clusters / Quantum Dots.

4. **Synthesis of Nanomaterial and Device Fabrication (10h)**
   - Synthesis of Bulk Polycrystalline Samples , Growth of Single Crystals, Synthesis Techniques for the Preparation of Nanoparticles, Requirements for Realizing Semiconductor Nanostructures, Specialized Growth Techniques for Nanostructures, Electrostatic-Induced Growth, Thermally Annealed Quantum Wells, Semiconductor Nano crystals.

5. **Different Types of Nanostructures (5 h)**
   - Shapes and Structures of Nanomaterial, Quantum Dots, Semiconductor Nanoparticles, Carbon Nanotechnology, Nanolithography

6. **Nanostructured Thin Films and Nanocomposites(5 h)**
   - Micro- and Nano scale Thin-Film Fabrication Techniques, Optical, Electrical, and Magnetic Properties of Nanostructured, Thin Films, Nano composites, Physical and Optical Properties, Metal/Dielectric-Organic Nano composites

7. **Nanoscale Characterization Techniques (8 h)**
   - Diffraction and Scherrer Method , Scanning Electron Microscopy, Transmission Electron Microscopy, Stoichiometry Study by Energy-Dispersive X-Ray Analysis, Scanning Probe Microscopy, Atomic Force Microscopy, X-Ray Photoelectron Spectroscopy, Diffuse Reflectance Spectra, Photoluminescence Spectra, Raman Spectroscopy, DC Magnetization, Electrical Resistivity Measurements, Theory of Linear Four-Probe Method.

8. **Recent Advances in Nanotechnology(2 h)**
   - Designing Molecules for Nanoelectronics, Advances of Nanotechnology in Materials Science

9. **Applications of Nanotechnology(5h)**
   - Applications in Material Science, Applications in Biology and Medicine, Applications in Surface Science, Applications in Energy and Environment , Applications of Nanostructured Thin Films, Applications of Quantum Dots, Applications of Magnetic Nanoparticles.

Books Recommended:

1. M.S. RamachandraRao, S. Singh, Nanoscience and Nanotechnology: Fundamentals of Frontiers, Wiley India. 2016.
2. G. Schmid, Nanoparticles: From Theory to Application, Wiley-VCH Verlag, 2005.
3. G. Cao, Y.Wang, Nanostructures and Nanomaterials Synthesis, Properties, and Applications 2^{nd} Ed. , World Scientific. 2004.

Semester IV
CH406: Advanced Bioinorganic Chemistry
Credits: 4(60h)

Course objective: The students will get advanced knowledge of role of metal ions in function of biological systems.

Learning outcome: Students will learn the role of metal ions in functioning of biological systems, toxicity due to metal ions, the role in a diseases and therapy.

1. **Metal ion storage and transport (7 h)**
   - Factors responsible for storage and transport of iron, Ferritin and Transferrin (structure & function). Biomineralisation of Fe, Si, P and Ca. Transport of Ca^{2+}.Active ion transport across cell membrane.

2. **Chemistry of dioxygen (12h)**
   - Review ofMössbauer, NMR and EPR in bioinorganic systems.Co-ordination of O_2/H_2O to metal centers and ligand/metal substitution.
   - Thermodynamics and kinetics of O_2 reactions with organic substrates. Detoxification enzymes – Catalases, Peroxidases, Superoxide dismutases. Coordination of O_2 to hemerythrin and hemocyanin (Raman spectroscopy)
   - Hemoglobinand its classical functional mimics. Water split reaction, conversion of O_2 into H_2O (respiration)

3. **Electron transport systems (12 h)**
   - Electronic coupling matrix.Marcustheory. Respiratory electron transfer chain – Energy storage &Release. Cytochrome c oxidase – spectroscopy & mechanism of O_2reduction.
   - Iron-Sulfur proteins – Spectroscopy, Magnetic properties, Model systems. Cytochrome c and modified cytochrome c. Plastocyanine.

4. **Metalloenzymes (15 h)**
   - Zinc enzymes: Useful characteristics of Zn(II) ion, Metal substitution in Zn enzymes, Carbonic anhydrase – structure, function, Co & Cu substitution studies, catalytic mechanism.
   - Carboxypeptidase – structure of active site, catalytic mechanism.
   - Monooxygenase: Cytochrome P 450 –structure, mechanism, porphyrin based model systems. Nitrogen fixation: Nitrogenases – structure, spectroscopy, N_2 activation and fixation, V-Nitrogenase, Model systems. V-peroxidase, Ni-hydrogenase

5. **Metal -Nucleic acid interaction (8h)**
   - Various types of interactions of metal complexes with DNA– coordination, intercalation, insertion, electrostatic & H-bonding. Interaction of tris(phenanthroline) Ru complex with DNA & monitoring techniques.
   - Applications of metal complex nucleic acid interactions. Interactions of cis-platin with DNA – evidence, kinetics, crosslinking reactions, biological consequences.
   - Photodynamic therapy-photocleavage of DNA by transition metal (Fe and Ru) complexes and its therapeutic implications.Oxidative stress due to iron and copper via Fenton mechanism and its consequences in human diseases.Inorganic nanoparticle in drug delivery.

6. **Metals in clinical radiology (6h)**
   - Gd-based MRI contrast agents, 99mTc and $BaSO_4$ (X-ray contrast agents)

Books Recommended:

1. Bioinorganic Chemistry – Bertini, Gray, Lippard, Valentine, Viva Books Pvt. Ltd., 1998
2. Bioinorganic Chemistry: A Short Course, R.M.Roat-Malone, Wiley Interscience
3. Biocoordination Chemistry, D.E. Fenton, Oxford University Press

Semester IV
CH407: Supramolecular Chemistry
Credits: 4(60h)

Course objective: Students will be introduced to the concepts/principles of supramolecular chemistry, receptor design, chemical and biochemical self-assembly, and catalysis.

Learning outcomes: Students will be able to classify/critically examine supramolecular systems, explicate the underlying principles, with regard to concepts of molecular recognition, self-assembly, catalysis, and devices.

1. Introduction to Supramolecular Chemistry(10 h)

- Definition of Supramolecular Chemistry, Biological Inspiration for Supramolecular Chemistry, Non-covalent interactions, Host-Guest interactions, Pre-organisation: Kinetic and Dynamic Effects, and complimentarity, lock and key analogy.

2. Synthesis, structure and their applications in recognitions(15 h)

- Crown ethers, podands, lariat ethers, cryptands, spherands, calixarenes, cyclodextrins, cyclophanes, cryptophanes, carcerands and hemicarcerands binding of organic and inorganic cationic, anionic, ion pair and neutral guest molecules with host molecules, Supramolecular chiral recognition, ion-transport in biological system.

3. Self-Assembly of molecules (10h)

- Design, synthesis and applications of metallomacrocycles, coordination polymers like Metal Organic Frameworks (MOFs), catenanes, rotaxanes, helicates and knots. Biochemical self-assembly. Surfactants, Micelles and Vesicles, Supramolecular Liquid Crystals.

4. **Supramolecular Catalysis (10 h)**

- Relevance of supramolecular chemistry to mimic biological systems: cyclodextrins as enzyme mimics, ion channel mimics, Corands as ATPase Mimics, abiotic supramolecular catalysis.

5. Molecular Devices (15h)

- Philosophy of molecular devices, Molecular and supramolecular photonic devices, Light conversion and energy transfer devices, Molecular and supramolecular electronic devices, Molecular wires, rectifiers, Molecular switches (Photo, electro, mechano, *etc.*), Molecular machines (gear, break, paddle wheel, shuttle *etc.*), Molecular and supramolecular electrochemical devices, supramolecular semiochemistry and sensing, Logic gates.

Recommended Books

1. K. Ariga, T. Kunitake, Supramolecular Chemistry–Fundamentals and Applications, Springer, 2006.
2. J. W. Steed, J. L. Atwood, Supramolecular Chemistry, 2nd Edition, **,** John Wiley & Sons, 2009
3. J-M. Lehn, Supramolecular Chemistry: Concepts and Perspectives, Wiley India Pvt. Ltd., 1995

Semester IV
CH408: Organometallic Chemistry
Credits: 4 (60 h)

Course objective: Students will be gain/develop insights into organometallic compounds/reagents, their application in organic synthesis and catalysis.

Learning outcome: Students will be able to discuss/explain the synthesis, structure, & reactivity of organometallic compounds, reagents, demonstrate/plan their use industrially important reactions.

1. **Review of organometallic compounds, and reaction mechanisms (5 h)**
   - Ligand substitution, oxidative addition, reductive elimination, migratory insertion, hydride elimination, trans-metallation, nucleophile and electrophilic attack on the ligands coordinated to metals.

2. **Physical methods in organometallic chemistry(15 h)**
   - Physical methods in organometallic chemistry: Characterization of organometallic molecules using NMR, EPR, Mössbauer , IR, Mass spectroscopy and X-ray crystallography; Isotope effect; Fluxionality of organometallic complexes. Characterization of aggregates of organolithium and organomercury compounds in solution using NMR.

3. **Main group organometallic compounds (15 h)**
   - Synthesis andreactions of Li, Mg, B, Al, Si, and Sn compounds: Synthetic applications in conjugate addition, allylic and propargylic substitution reactions; Hydrostannation reaction; Examples of applications in C-C bond forming reactions

4. **d-block organometallic compounds (15 h)**
   - Structure and bonding of d-block organometallic compounds, 18e-rule in organometallic structure prediction and the limitations.
   - Catalysis using metal cluster; Nitrogen activation.
   - Dötz reaction, Heck, Stille, Suzuki, Negishi and Sonogashira, Nozaki-Hiyama, Buchwald-Hartwig, Ullmann coupling reactions, directed *ortho*-metalation. Metal (Rh, Ir) catalyzed C-H activation reactions and their synthetic utility.
   - Organometallic compounds of imidazole, purine, porphyrine, Tris(pyrazolyl)borate; Vit B_{12}
   - Bio-medical applications of organometallic compounds.

5. **Organometallic catalysis (10 h)**
   - Synthetic applications of metathesis reactions, ring opening, ring closing metathesis in organic synthesis, macrocycles synthesis
   - Fischer, Schrock and Grubbs type carbene complexes (review).
   - Cu- and Rh-based carbene and nitrene complexes, Reactions of carbene complexes and their synthetic utility; Cyclopropanation, Rh-catalysed C-H insertion and aziridination reactions including asymmetric version. Introduction to N-heterocyclic carbene metal complexes as catalysts.

Books Recommended:

1. C. Elschenbroich, Organometallics, 3rd Edition, Wiley, 2006.
2. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals,6th Rev. Edition , Wiley-Blackwell, 2014.
3. M. Bochmann, Organometallics and Catalysis: An Introduction, Oxford University Press, 2014.
4. M. B. Smith, Organic Synthesis, 2ndEdition, McGraw Hill Higher Education, 2005.

Semester IV
CH409: Medicinal Chemistry
Credits: 4 (60 h)

Course objective: Studentswill be introduced to various types of drugs and medicines, their chemistry, mode of action and theoretical aspects of drug design and action.

Learning outcome: Students will be able to identify, compare and explain aspects related to drug design, drug action and SARs.

1. Introduction & History of Drug Development(4 h)

- Definition of drug and prodrugs, need of drugs, germ theory of diseases, history of sulpha drugs & their mode of action, about antibacterial agents.

2. Basic Concepts of Mechanism of Drug Action (6 h)

- About receptors and the two-state model of receptor theory, drug-receptor interaction and Clark's Occupancy Theory, physiological response, drug agonist & antagonist and their classification.

3. Theoretical Aspects of Drug Action (6 h)

- Need of quantification of drug action, definition of chemotherapeutic index & therapeutic index, factors affecting bioactivity of drugs, pharmacokinetics and pharmacodynamics, QSAR.

4. Drug Discovery and Design (6 h)

- About lead compounds in drug discovery, importance of SAR & molecular modification, importance of combinatorial library and molecular modeling in drug discovery, introduction to gene therapy.

5. Antibiotics - A Major Group of Drugs (18 h)

- Definition of antibiotics, their sources and classification, causes & concerns of bacterial resistance to antibiotics, Definition and need of broad spectrum antibiotics.
- History leading to the discovery of penicillins (β-lactam antibiotics) – natural & semi-synthetic penicillins, structure activity relationship & chemical modification, bacterial resistance to penicillins - causes and inhibitors, mode of action of β-lactam antibiotics, origin of high reactivity of penicillins and related consequences.
- Aminoglycoside antibiotics, their sources and uses, streptomycin, gentamycin, kanamycin, neomycin and their SAR & mode of action.
- Importance of teracyclines& chloramphenicol as broad spectrum antibiotics, their therapeutic uses and structure activity relationship, mode of action.
- Introduction to macrolide antibiotics: ansa& lactone macrolides, peptide antibiotics (toxicity and limitation).

6. Antimalarials (10 h)

- Classification of human malaria and plasmodia responsible for human malaria, Discovery of quinine and its SAR, importance of quinine as a lead to discovery of other low cost antimalarials, artemisinin and its derivatives, their SAR and importance in dealing with CQ resistant malaria, mode of action.

7. Introduction to Viral Diseases & Treatment (5 h)

- Difficulty in developing clinical solution to viral diseases, introduction to antiviral agents, AIDS – its cause and prevention

8. Drugs for Treatment of Cancer (5 h)

- Cancer and its causes, difficulty in developing clinical solution, chemotherapy of cancer – uses of vinca alkaloids, taxol and its derivatives

Books Recommended:

1. G. Thomas, Medicinal Chemistry: An Introduction, 2nd Edition. John Wiley & Sons, 2007
2. G. L. Patrick,An Introduction to Medicinal Chemistry, 5th Edition. , Oxford University Press, 2013.
3. A. Gringauz, Introduction to Medicinal Chemistry, Wiley India Pvt Ltd, 2010.

Semester IV
CH410: NMR methods for structure elucidation
Credit: 4(60h)

Course objective: Figuring out the chemical structure of a molecule from scratch is an essential part of researching chemicals that come from nature, or "natural products." NMR has recently become a powerful tool to determine their structures. This course is designed to familiarize students with NMR spectroscopy as a tool for molecular structure determination (both organic/inorganic), for conformation analysis, and to assign relative and absolute configuration of chiral natural products.

Leaning outcome: Student will be able to apply/interpret NMR methods for structure elucidation of complex molecules.

1. Introductory NMR spectroscopy (10h)

- Review of NMR techniques, Isotropic NMR parameters-chemical shifts and *J*-couplings and Nuclear Overhauser effect (NOE). Anisotropic NMR parameters.

2. Alignment media(10h)

- Importance of alignment media – liquid crystals (PBLG and DNA), aligning gels (PMMA, poly-HEMA). NQR (only deuterium NMR), Deuterium splitting

3. Applications of 2D NMR (10 h)

- Introduction to 2D - NMR. Assignment of ^{1}H and ^{13}C chemical shifts by using 2D COSY, HSQC and HMBC spectra for simple organic molecules and natural products.

4. Structure elucidation for organic natural products (10h)

- Determination of 2D structure or constitution; Conformation and relative configuration of chiral organic natural products by using NMR data; Determination of absolute configuration based on NMR data and circular dichroism/optical rotatory dispersion.

5. Structure elucidation for inorganic complexes/materials (20h)

- NMR of paramagnetic metal complexes-contact shifts and pseudo-contact shifts; solid state NMR applications to determine the crystal structure of drugs.^{19}F, ^{31}P NMR in metal organic frameworks, $^{6/7}$Li NMR in organometallic compounds and ^{29}Si NMR in zeolites.

Books Recommended:

1. D. L. Pavia, G. M. Lampman, G. S. Kriz, Introduction to Spectroscopy, 4th Edition, Cengage, 2001
2. J. Keeler, Understanding NMR spectroscopy, 2nd Edition, Wiley.
3. J. R. Kalman, L. D. Field, S. Sternhell Organic Structures from Spectra, 4th Edition, Wiley.
4. G. Kummerlöwe, B. Luy, Residual dipolar couplings for configurational and conformational analysis of organic molecules, Annual Reports on NMR Spectroscopy, 2009.

Semester IV
CH411: Project Dissertation
Credit: 12

Course objective:

This purpose is to train students with various stages of research planning and implementation. Students are expected to perform scientific research under the Faculty supervisor, and learn to work independently.

During the course of her/his project work, students are expected to learn different methods and techniques for carrying out scientific research problems, particularly to collect and interpret data.

Students will also learn to survey research literature, and collect/compile the information for preparing reports and for publications.

Learning outcome:

Following the completion of this course, students should be able demonstrate ability to plan and strategize a scientific research problem, and implement it within a reasonable time-frame. It is expected that after completing this project dissertation, students will learn to work independently and how to keep accurate/readable record of their experimental work.

In addition, students will be able to handle laboratory equipment and chemicals. Also, students will be able to utilize sophisticated instruments for analysis, data collection and interpretation.

Subsequently, the students should be able to critically examine research articles, and improve their scientific writing/communication skills.