Course Structure and Detailed Syllabi of M. Sc. (Chemistry)

Starting Year: 2018, Autumn Semester

(Revised)

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Department of Chemical Sciences

(DST-FIST and UGC-SAP DRS-II SUPPORTED)

TEZPUR UNIVERSITY

Preamble

The course structure of M.Sc. in Chemistry is a two-year post-graduation program of Tezpur University. The course offered through this curriculum, would allow students to grow fundamental knowledge of chemical sciences and specialize them for careers in chemistry with high scientific depth and temperament. The concept based learning of fundamental properties of chemical processes, synthetic methods of chemical compounds and development of experimental skills, understanding of sustainable development process and implementation of novel synthetic routes, acquiring structure elucidation techniques, understanding of biological processes, uses of computational chemistry to study the interactions at sub-atomic, atomic and molecular levels and also towards computer assisted drug designing are among such important aspects of the basic structure. The programme follows UGC's Choice Based Credit System (CBCS). The Choice Based Credit System (CBCS) provides an interdisciplinary approach in learning and enables students to learn at their own pace to complete a programme of study, choose electives from a wide range of courses across departments/centres/institutions, study add on courses and acquire more than required number of credits. In CBCS system the courses are divided into three main categories viz. Core Courses, Elective Courses and Ability Enhancement Courses. Each course is assigned with a fixed number of credits based on the contents to be learned. The number of credits earned by the student reflects the knowledge or skill acquired by them. For assessment of student's continuous comprehensive evaluation shall be followed to reduce the weightage on the semester-end examination so that students enjoy a de-stressed learning environment. The grade points earned for each course reflects the student's proficiency in in that course.

1. Introduction

The main objective of this programme are to impart the key knowledge of chemical sciences and expertise to prepare students for careers in chemistry with high scientific depth and temperament and to prepare quality postgraduates for further research and development and entrepreneurship. The eligibility criteria for enrolment in the M.Sc. in Chemistry programme is Bachelor‘s Degree with minimum 45% marks in Major/Honours in Chemistry, or 50% marks in Chemistry as well as in aggregate if not having Major/Honours in Chemistry. Also, candidates should have Physics and Mathematics as subsidiary Subjects in Bachelor‘s Degree. Reservation and relaxation will be as per the government rules. The M.Sc. in chemistry programme comprises four semesters course spread over two academic years. The total credit requirement to acquire the M.Sc. degree is 80 credits.

The curriculum for the M.Sc. in Chemistry programme is based on learning outcome based curriculum framework (LOCF). The syllabus contains core as well as elective courses which are mostly Discipline specific. The program structure provides an opportunity to a student to choose any elective courses from the syllabus comprising of different elective courses. The syllabus offers a flexibility of programme structure while ensuring that students get a strong foundation and gains in-depth knowledge in chemistry. The LOCF strategy gives students a clear view to focus their learning effort and enable them to make a choice of the elective courses they prefer to study. The syllabus fulfils the current needs to acquire a good chemistry degree and to secure a good choice in higher education in chemistry and the area of their interest as well as employment.

2. Qualification descriptors for the graduates

Knowledge & Understanding:

- Gains comprehensive knowledge and understanding on fundamental principles and concepts chemical sciences that covers the sub-disciplines (Physical, Inorganic, Organic) as well as advanced and emerging topics.

- Able to apply underlying ideas and principles outside the context in which they were first studied and in interdisciplinary problems and circumstances.

Skills and Techniques:

- Exhibition of skills required for conducting the documented laboratory procedure as well as developed skills for the planning new experiments, data analysis and presentation of quantitative and/or qualitative data or information, ideas, concepts etc.
- Acquisition of skills in the handling of chemicals and operation of standard instruments.
- Development of information searching and management skills

Competence:

- Acquisition of competence in the use of routine materials, techniques and practices of chemistry
- Development of competence in intellectual, practical, IT skills and Communication skills necessary for employment as professional chemist.
- Development of responsibilities of the uses of chemistry in everyday life.

2. Graduate Attributes

- Students will be able to clearly communicate the results of scientific work in oral, written and ICT formats to both science community and society.
- Students will be able to explain why chemistry is an integral activity for addressing social, economic, and environmental problems.
- Students will learn to act with integrity and good ethics in their profession and their obligation to society.
- Students will be able to demonstrate knowledge and skills in analyzing and identifying entrepreneur opportunities.

4. Program Outcomes

PO 1. Students will have a firm foundation in the fundamentals and application of current chemical and basic science including those in Physical, Organic, Inorganic, Analytical and Chemistry of life.

PO 2. Students will have high awareness of major issues and development of chemical research and competent in initiating, developing, and pursuing a scientific research.

PO 3. Students will be able to seek new knowledge, skills and manage relevant information from various sources.

PO 4. Students will be trained to work effectively and safely in the laboratory environment. Students will learn to work in teams as well as independently.

PO 5. Students will be able to design and carry out scientific experiments as well as accurately draw logical inferences from the results of such experiments.

5. Programme structure

Total Credits: 80

Structure of the curriculum:

Course Category	**No of courses**	**Credits per course**	**Total Credits**
I. Core courses	**17**	**3/6/8**	**65**
II. Elective courses			
Discipline Specific Elective (DSE) courses	**05**	**03**	**15**
Total credits			**80**

6. SEMESTER-WISE SCHEDULE

SEMESTER I

Course type	Course title	Lecture (L)	Tutorial (T)	Practical (P)	Contact Hour (CH)	Credits
Core	CH 401: Principles of Inorganic Chemistry	3	0	0	3	3
	CH 403: Chemical and Statistical Thermodynamics	3	0	0	3	3
	CH 407: Principles of Organic Chemistry	3	0	0	3	3
	CH 409: Quantum Chemistry and Chemical Bonding-I	3	0	0	3	3
	CH 411: Principles and Applications of Spectroscopy	3	0	0	3	3
	CH 405: Laboratory Course in Organic Chemistry	0	0	6	12	6

SEMESTER II

Course type	**Course title**	**Lecture (L)**	**Tutorial (T)**	**Practical (P)**	**Contact Hour (CH)**	**Credits**
Core	CH 408: Chemistry of Transition Elements	**3**	**0**	**0**	**3**	**3**
	CH 410: Chemical Dynamics and Electrochemistry	**3**	**0**	**0**	**3**	**3**
	CH 414: Quantum Chemistry and	**3**	**0**	**0**	**3**	**3**

	Chemical Bonding-II					
	CH 412: Laboratory Course in Inorganic Chemistry	**0**	**0**	**6**	**12**	**6**
	CH 418: Organic Reactions and Mechanism	**3**	**0**	**0**	**3**	**3**
Discipline Specific Elective	CH 416: History of Chemistry	**3**	**0**	**0**	**3**	**3**

SEMESTER III

Course type	**Course title**	**Lecture (L)**	**Tutorial (T)**	**Practical (P)**	**Contact Hour (CH)**	**Credits**
Core	CH 501: Bio-Organic Chemistry	3	0	0	3	3
	CH 519: Physical Chemistry of Surface and Condensed Systems	3	0	0	3	3
	CH 521: Analytical Methods in Chemistry	3	0	0	3	3
	CH 525: Organometallic Chemistry	3	0	0	3	3
	CH 505: Laboratory Course in Physical Chemistry	0	0	6	12	6
Discipline Specific Elective	CH 523: Chemical Technology and Society	3	0	0	0	3

SEMESTER IV

Course type	Course title	Lecture (L)	Tutorial (T)	Practical (P)	Contact Hour (CH)	Credits
Core	CH 530: Project Work*	**0**	**0**	**8**	**16**	**8**
Elective I (Discipline Specific Elective**)**	CH 506: Catalysis / CH508: Methods in Organic Synthesis / CH528: Special Topics in Inorganic Chemistry / CH532: Chemistry of Paints and Surface Coating	**3**	**0**	**0**	**3**	**3**
Elective II(Discipline Specific Elective**)**	CH 514: Biomolecular Chemistry/ CH516: Computational Chemistry and Numerical Analysis / CH518: Organic Solid States Chemistry / CH520: Environmental and Green Chemistry / CH534: Industrial Polymer	**3**	**0**	**0**	**3**	**3**
Elective III (Discipline Specific Elective**)**	CH 522: Polymer Chemistry / CH524:Heterocyclic Compounds and Medicinal Applications / CH526:Bio-inorganic Chemistry / CH536: Chemistry of Materials	**3**	**0**	**0**	**3**	**3**

*** To be carried out in the Department under the guidance of an assigned faculty member of the Department.**

7. Mapping of course with program outcomes (POs)

Course title	PO1	PO2	PO3	PO4	PO5
CH 401: Principles of Inorganic Chemistry	✓	✓	✓		✓
CH 403: Chemical and Statistical Thermodynamics	✓	✓	✓		✓
CH 407: Principles of Organic Chemistry	✓	✓	✓		✓
CH 409: Quantum Chemistry and Chemical Bonding-I	✓	✓	✓		✓
CH 411: Principles and Applications of Spectroscopy	✓	✓	✓		✓
CH 405: Laboratory Course in Organic Chemistry	✓	✓	✓	✓	✓
CH 408: Chemistry of Transition Elements	✓	✓	✓		✓
CH 410: Chemical Dynamics and Electrochemistry	✓	✓	✓		✓
CH 414: Quantum Chemistry and Chemical Bonding-II	✓	✓	✓		✓
CH 412: Laboratory Course in Inorganic Chemistry	✓	✓	✓	✓	✓
CH 418: Organic Reactions and Mechanism	✓	✓	✓		✓
CH 416: History of Chemistry	✓	✓	✓		✓
CH 501: Bio-Organic Chemistry	✓	✓	✓		✓
CH 519: Physical Chemistry of Surface and Condensed Systems	✓	✓	✓		✓
CH 521: Analytical Methods in Chemistry	✓	✓	✓	✓	✓
CH 525: Organometallic Chemistry	✓	✓	✓		✓
CH 505: Laboratory Course in Physical Chemistry	✓	✓	✓	✓	✓
CH 530: Project Work		✓	✓	✓	✓
CH 523: Chemical Technology and Society	✓	✓	✓		✓
CH 506: Catalysis Synthesis	✓	✓	✓		✓
CH508: Methods in Organic	✓	✓	✓		✓
CH528: Special Topics in Inorganic Chemistry	✓	✓	✓		✓
CH532: Chemistry of Paints and Surface Coating	✓	✓	✓		✓
CH 514: Biomolecular Chemistry	✓	✓	✓		✓

CH516: Computational Chemistry and Numerical Analysis	✓	✓	✓	✓	✓
CH518: Organic Solid States Chemistry	✓	✓	✓		✓
CH520:Environmental and Green Chemistry	✓	✓	✓	✓	✓
CH 534: Industrial Polymer	✓	✓	✓	✓	✓
CH 522: Polymer Chemistry	✓	✓	✓		✓
CH524:Heterocyclic Compounds and Medicinal Applications	✓	✓	✓		✓
CH526:Bio-inorganic Chemistry	✓	✓	✓		✓
CH536: Chemistry of Materials	✓	✓	✓		✓

8. Evaluation plan

Students shall be evaluated separately in each course through a Continuous Comprehensive Evaluation (CCE) system as mentioned in the academic guideline of Tezpur University.

9. DETAILED SYLLABUS

CH 401 PRINCIPLES OF INORGANIC CHEMISTRY L3 T0 P0 CR3

Course outcomes:

On completion of this course the students will be able to understand:

CO1: Periodic properties of elements including lanthanides

CO2: Valence bond, molecular orbital theory and VSEPR model of inorganic systems

CO3: Fundamentals of group theory, Application of group theory in predicting the IR and Raman active vibrational modes, orbital symmetry and chemical reactions

CO4: Trace and essential metals in biological systems

CO5: Sodium potassium pump, heme and non-heme proteins and their biological importance

Course Content:

Unit 1 **[10 Lectures]**

Brief review of the following: Periodic properties, lanthanide contraction, ionic bonding, valence bond theory and LCAO-MO theory, orbital symmetry and overlap, bond energy and covalent radii, VSEPR model and Walsh diagram, Introduction to non-covalent interaction.

Unit 2 **[16 Lectures]**

Group theory: Symmetry elements and symmetry operations, symmetry groups, molecular dissymmetry and optical activity, symmetry point groups for compounds having co-ordination number 2 to 9, Historical development of Evariste Galois theory of groups, matrix representation of groups, reducible and irreducible representation, the great orthogonality theorem, Direct product representation. Projection operator, symmetry adapted linear combination, vibrational modes as bases for group representation, symmetry selection rules for IR and Raman spectra, orbital Symmetry and Chemical reactions –Woodward and Hoffman rules for electrocyclic and cycloaddition reactions.

Unit 3 **[10 Lectures]**

Bioinorganic chemistry: scope, inorganic elements in biological systems, basic bioenergetics, active transport of cations across membranes, Na^+/K^+ pump, heme-protiens–haemoglobin and myoglobin: structure, thermodynamics and kinetics of oxygenation, Cytochrome P_{450}, Hemerythrin, Ferritin and Transferrin.

Text Book(s)

1. Cotton, F. A., Wilkinson, G., Murillo, C. A. and Bochmann, M. *Advanced Inorganic Chemistry*, 6th Edn., (John Wiley, 2007).
2. Huheey, J. E., Keiter, E. A., Keiter, R. L. and Medhi, O. K. *Inorganic Chemistry*: Principles of *Structure and Reactivity*, 4th Edn., (Pearson Education, 2006).

Reference Book(s)

1. Cotton, F.A., *Chemical Application of Group Theory,* 3rd Edn., (John Wiley & Sons, 2008).
2. Bertini, I., Gray, H. B., Lippard, S. J. and Valentine, J. S. *Bioinorganic Chemistry,* (Viva Books Pvt. Ltd. 2004).

CH 403: CHEMICAL AND STATISTICAL THERMODYNAMICS L 3 T0 P0 CR 3

Course outcomes:

After completion of the course, the learner shall be able to understand:

CO1: Fundamentals of equilibrium thermodynamics

CO 2: Thermodynamics of phase transition and phase diagrams

CO3: Basics of statistical thermodynamics

CO4: Basics of non-equilibrium thermodynamics

Course Content:

Unit 1 [12 Lectures]

Brief review of thermodynamic functions and laws of thermodynamics: Temperature dependence of thermodynamic functions, Experimental determination of thermodynamic functions, Thermodynamic description of mixtures, Gibbs-Duhem equation, Chemical equilibrium, Thermodynamic description of phase transitions, Clapeyron-Claussius equation, Phase diagrams, Thermodynamics of nonideal systems – fugacity and activity concepts, excess properties.

Unit 2 **[12 Lectures]**

Concepts of statistical thermodynamics, entropy and probability, ensembles, distribution laws of MB, FD and BE, partition functions and statistical formulation of macroscopic variables. Use of statistical thermodynamics including calculation of electrical and magnetic properties, and heat capacity of solids, application of BE statistics to helium.

Unit 3 **[12 Lectures]**

Non-equilibrium thermodynamics, thermodynamic criteria for non-equilibrium states, Assumptions of non-equilibrium thermodynamics, uncompensated heat, entropy production and entropy flow, entropy balance, Onsager formalism, relation between forces and fluxes, transformations of generalized fluxes and forces, microscopic reversibility and Onsager's reciprocity relations.
Electrokinetic phenomena, diffusion, electric conduction, irreversible thermodynamics for biological systems, coupled reactions.

Text Book(s)

1. Engel, T. and Reid, P. *Thermodynamics, Statistical Thermodynamics and Kinetics,* 2nd Edn., (Pearson, New Delhi, 2011).
2. Kalidas, C. and Sangaranarayanan, M.V. *Non-equilibrium Thermodynamics, Principles and applications,* (Mcmillan, New Delhi, 2002).

Reference Book(s)

1. Atkins, P. and Paula, J. de. *Atkins' Physical Chemistry*, 10*th* Edn., (Oxford University Press, New Delhi, 2014).
2. Berry, R. Rice S. A. and Ross, J. *Physical Chemistry,* 2nd Edn*.,* (Oxford, London, 2010***).***

CH 407: PRINCIPLES OF ORGANIC CHEMISTRY L 3 T 0 P0 CR 3

Course outcomes:

After completion of the course, the learner shall be able to understand:

CO1: Understanding of structure-activity relationship of organic molecules.

CO2: Stereochemistry of organic molecules, prostereogenic elements and asymmetric synthesis.

CO3: Basic concepts of nucleophilic substitution, elimination, addition and neighbouring group participation reactions with stereochemical outcomes of products.

CO4: Chemistry of five, six and fused heterocyclic compounds

Course content:

Unit 1 [4 Lectures]

Structure and Bonding: Reactivity of organic molecules, aromaticity, n-annulenes and hetero-annulenes, fullerenes (C_{60}), Graphene, Cryptans, bonds weaker than covalent: addition compounds, inclusion compounds and rotaxenes.

Unit 2 [3 Lectures]

Thermodynamics and Kinetics: Acids and bases, concept of hard and soft acids and bases, symbiosis, labeling and kinetic isotope effects, Hammett equation, σ–ρ relationship, non-classical carbenuim ion (or carbocation), kinetic and thermodynamic control, Hammand principle, Curtin-Hammett principle, transition state and intermediates.

Unit 3 [10 Lectures]

Stereochemistry: Chirality and isomerism in organic system, conformational analysis of simple cyclic and acyclic systems, conformation of saturated heterocycles, interconversion of Fischer, Newman and Sawhorse formula, *E-Z* isomerism, *R-S* nomenclature, diastereomerism in acyclic and cyclic systems, newer methods of asymmetric synthesis (including enzymatic and catalytic nexus), enantio-, and diastereo selective synthesis, determination of enantiomeric and diastereomeric excess, stereospecific synthesis, effect of conformation on reactivity, methods of resolution, optical purity, optical activity in absence of chiral atom, neighbouring group participation reactions and examples involving non-classical carbocation.

Unit 4 **[8 Lectures]**

General reaction mechanism, aliphatic substitution reaction, S_N1, S_N2, mixed S_N1 and S_N2 and S_Ni reaction, SET reaction, classical and nonclassical carbocations, electrophilic substitution reaction, S_E1, S_E2, S_Ei mechanism, electrophilic and nucleophilic aromatic substitution reaction, SNAr, Benzyne, SRN^1 mechanism, reactivity, effect of substrate, leaving group and attacking nucleophile, elimination reaction, E^1 E^2 and E^1Cb, protection-deprotection chemistry of selected functional groups such as aldehydes, ketone and –OH, NH_2.

Unit 5 **[6 Lectures]**

Addition Reaction: Mechanism and stereochemical aspects of addition reaction in carbon-carbon multiple bonds, region and chemoselectivity, orientation and reactivity, mechanism of condensation reactions involving enolates- Aldol, cross Aldol, Knoevenagel, Claisen, Perkin and Stobbe reactions.

Unit 6 **[5 Lectures]**

Heterocyclic Chemistry: π-excessive and π-deficient heterocycles, synthesis, reactions and reactivity of heterocycles, e.g. furan, thiophene, pyrrole, pyridine, pyrazoles, pyridazines, pyrimidines, isoxazoles, tetrazoles, quinoline, isoquinoline and indole, Skraup synthesis, Fischer-Indole synthesis, Vilsmeyer-Heck formylation reaction.

Text Book(s)

1. Carey, F. A., Sundberg, R. J. *Advanced Organic Chemistry, Part A: Structure and Mechanisms,* 5th Edn., (Springer, New York, 2007).

2. Clayden, J., Greeves, N., Warren, S., Wothers, P. *Organic Chemistry*, 2nd Edn., (Oxford University Press, 2012).
3. March, J., Smith, M. B. *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, 6th Edn., (Wiley, 2007).
4. Sengupta, S. *Basic Stereochemistry of Organic Molecules*, 1st Edn., (Oxford University Press, 2014).
5. Kalsi, P. S. *Stereochemistry, Conformation and Mechanism*, (New Age international Publishers, 2009).
6. Finar, I. L. *Organic Chemistry* (Volume 1), 6th Edn., (Pearson Education, 2002).

Reference Book(s)

1. Sykes, P. *A Guide Book to Mechanism in Organic Chemistry,* 6th Edn., (Longman, 1986).
2. Carey, F. A., Sundberg, R. J. *Advanced Organic Chemistry, Part B: Reactions and Synthesis,* 5th Edn., (Springer, New York, 2007).
3. Eliel, E. L., Wilen, S. H., Doyle, M. P. *Basic Organic Stereochemistry*, 1st Edn., (Wiley-Interscience, 2001).
4. Zweifel, G. S., Nantz, M. H., Somfai, P. *Modern Organic Synthesis: An Introduction*, 2nd Edn., (Wiley, New York, 2017).

CH 409: QUANTUM CHEMISTRY AND CHEMICAL BONDING-I L 3 T 3 P0 CR 3

Course outcomes:

After completion of the course, the learner shall be able to learn:

CO1: Basic mathematics involved in quantum chemistry

CO2: Origin of quantum chemistry

CO3: The solution of the Schrodinger equation for different model systems and their correlation with real systems

CO4: Approximate methods used in the solution of Schrodinger equations

Course Content:

Unit 1 **[10 Lectures]**

Mathematical Review: Basic vector algebra, matrix, determinant, eigen value equations, quantum mechanical operators, orthogonal functions, Schmidt's orthogonalization technique.

Unit 2 **[14 Lectures]**

Planck's quantum theory, wave-particle duality, uncertainty principle, postulates of quantum mechanics, Schrödinger equation, free particle, particle in a box, degeneracy, harmonic oscillator, rigid rotator, the hydrogen atom, angular momentum, electron spin, spin-orbit coupling.

Unit 3 **[12 Lectures]**

Approximate methods in quantum mechanics: The variation theorem, linear variation principle and perturbation theory (first order and non-degenerate), application of variation method and perturbation theory to the Helium atom, antisymmetry, Slater determinant, term symbols and spectroscopic states.

Text Book(s)

1. Atkins, P. W., Friedman, R. S., *Molecular Quantum Mechanics*, (Oxford University Press, 1997).
2. Levine, I. N *Quantum Chemistry*, (Pearson Education, 2004).

Reference Book(s)

1. McQuarrie, D. A. *Quantum Chemistry* 2^{nd} Edn., (University Science Books, 2007).
2. Prasad, R. K. *Quantum Chemistry* (New Age, 2010).

CH 411: PRINCIPLES AND APPLICATIONS OF SPECTROSCOPY **L 3 T 3 P 0 CR 3**

Course outcomes:

On completion of this course the students will be able to understand:

CO1: Basic principles of spectroscopy, interaction of electromagnetic radiation with matter, atomic and molecular spectroscopy

CO2: Selection rules and allowed transitions, factors effecting the molecular and electronic transitions

CO3: Different laws and principles like Beer-Lamberts Law, Frank-Condon principle, Woodward-Fieser rules, Raman Effect, Mössbuer effect, Mc-Lafferty rule etc.

CO4: Different spectroscopic parameters like absorption wavelength, peak intensity, peak half width, chemical shift value, g-value, isomer shift value

CO5: Basic principles and instrumentation of various spectroscopic techniques viz FTIR, Raman, UV-vis, NMR including 2D, ESR, Mössbauer spectroscopy and Mass spectrometry

Course Content:

Unit 1 **[8 Lectures]**

Rotational and Vibrational spectra: Basic principles, selection rule, fundamental vibrations, Raman effect, identification of some representative organic and inorganic compounds.

Unit 2 **[5 Lectures]**

Electronic spectra: Frank-Condon principle, Fluorescence, Phosphorescence, electronic spectra of diatomic molecules, chromophores, auxochromes, absorption and intensity shifts, solvent effects, Woodward Fieser rules.

Unit 3 **[10 Lectures]**

Nuclear Magnetic Resonance Spectroscopy: Basic principles, origin of chemical shifts, factors affecting the chemical shifts and their interpretation, spin-spin coupling, relaxation processes, coupling constants, Nuclear Overhouser effect (NOE) 2D-NMR, DEPT, HMQC, HMBC, ^{1}H, ^{13}C, ^{31}P, ^{15}N and ^{19}F NMR spectra of selected compounds, Shift reagents, spin tickling.

Unit 4 **[3 Lectures]**

Mass spectrometry: Basic principles and instrumentation, mass spectral fragmentation of organic compounds, applications to organometallic compounds.

Unit 5 **[5 Lectures]**

EPR spectroscopy: Basic principles, origin of g-shifts , hyperfine and super hyperfine coupling, spin orbit coupling, line shape, zero field splitting, Kramer degeneracy, ESR analysis of organic compounds, transition metal complexes of vanadium, copper, cobalt and iron.

Unit 6 **[5 Lectures]**

Mössbauer spectroscopy: Nuclear resonance absorption, recoil energy, Doppler effect, Mössbauer effect, Isomer shift, quadruple interactions, effect of magnetic field, determination of oxidation states of iron (including bioinorganic systems, ferredoxins) tin and cobalt compounds.

Text Book(s)

1. Banwell, C. N., McCash, E. M. *Fundamentals of Molecular Spectroscopy*, (Tata McGraw Hill, 1994).
2. Pavia, D. L., Lampman, G. M., Kriz, G. S., Vyvyan, J. R. *Introduction to Spectroscopy*, (Cengage India, 2015)

Reference Book(s)

1. Drago, R. S. *Physical Methods for Chemistry*, (Saunders Company, 1992).
2. Nakamoto, K. *Infrared and Raman Spectra: Inorganic and Coordination Compounds,* 6^{th} Edn., (John Wiley, 2009).
3. Dutta, R. L. & Syamal, A. *Elements of Magnetochemistry,* 2^{nd} Edn., (East West Press,1993).

CH 405: LABORATORY COURSE IN ORGANIC CHEMISTRY L 0 T 0 P 6 CR 6

Unit 1

Separation techniques of organic compounds and their spectroscopic identification.

Experiments involving the separation and purification of organic compounds from a mixture, using chromatographic techniques, steam distillation, fractional crystallization and sublimation.

Unit 2

Synthesis of organic compounds using common reagents: At least eight preparation (involving two or more than two steps) involving the following representative reactions: (a) Oxidation of alcohol, (b) Reduction of carbonyl group, (c) Nucleophilic substitution, (d) Cycloaddition reaction, (e) Condensation reaction, (f) Aromatic electrophilic substitution, (g) Preparation of dyes, (h) Heterocyclic synthesis, (i) Solid phase synthesis etc.

Unit 3

Natural product extraction: Caffeine, Nicotine, Carotenoids etc.

Unit 4

Estimation of Glucose, acetic acid in vinegar, -OH groups etc.

Unit 5

Determination of acid value and saponification value of fat/oil.

Unit 6

Green experiments

Text Book(s)

1. Pasto, D., Johnson, Miller, M. *Experiments and Techniques in Organic Chemistry*, (Prentice Hall, 1992).

2. Williamson, K. L. *Macroscale and Microscale Organic Experiments*, (D. C. Heath & Company, 1999).

Reference Book(s)

1. Furniss, B. S., Ford, A. J. H., Smith, P. W. H., Tatchell, A. R. *Vogel's Textbook of Practical Organic Chemistry,* 5^{th} Edn., (Wiley, 1989).

CH 408: CHEMISTRY OF TRANSITION ELEMENTS L 3 T 0 P 0 CR 3

Course outcomes:

On completion of this course the students will be able to understand:

CO1: Crystal Field and Ligand Field theory of transition metal complexes

CO2: Charge transfer transition, and optical properties of metal complexes

CO3: Kinetic and thermodynamic stability of metal complexes, stability constants

CO4: Reaction mechanism of square and octahedral complexes, trans effect, outer and inner sphere mechanism in metal complexes

CO5: Magnetism, Magnetic Properties of transition metal complexes and lanthanides

Course Content:

Unit 1 [12 Lectures]

Electronic structure and spectra of transition metal complexes: Spectroscopic states, Crystal Field Theory, Orgel and Tanabe-Sugano diagrams, selection rules, band intensities and band width, Adjusted Crystal Field Theory, Spectrochemical and Nephelauxetic series, molecular orbital theory of complexes (including complexes with and without π bonding), MO diagrams for octahedral and tetrahedral complexes, Jahn-Teller effect, Charge-transfer spectra, optical properties of lanthanides and actinides.

Unit 2 [10 Lectures]

Magnetic properties of transition metal complexes: Types of magnetic behaviour: dia-, para-, ferro- and anti-ferromagnetic compounds, spin-orbit coupling, temperature independent paramagnetism, application of Crystal Field Theory to explain magnetic properties, spin-crossover. Thermodynamic effects-hydration, ligation, lattice energy, magnetic properties of lanthanides and actinides.

Unit 3 **[14 Lectures]**

Reaction Mechanism of inorganic complexes: Stepwise and overall formation constants. Factors affecting the stability of metal complexes, chelate effect, determination of binary formation constants, Energy profile of a reaction, inert and labile complexes, kinetics of substitution in octahedral complexes, acid hydrolysis and base hydrolysis. Dissociative, associative and interchange mechanism, trans-effect, isomerisation and racemisation in tris-chelate complexes, electron-transfer reactions, stereo-chemical non-rigidity and fluxional molecules.

Text Book(s)

1. Huheey, J. E., Keiter, E. A., Keiter, R. L. and Medhi, O. K. *Inorganic Chemistry*: Principles of *Structure and Reactivity*, 4th Edn., (Pearson Education, 2006).
2. Cotton, F. A., Wilkinson, G., Murillo, C. A. and Bochmann, M. *Advanced Inorganic Chemistry*, 6th Edn., (John Wiley, 2007).

Reference Book(s)

1. Greenwood, N. N., Earnshaw, A. *Chemistry of the Elements,* 2nd Edn., (Pergamon Press, 1997).
2. Carlin, R.L. *Magnetochemistry*, (Springer Verlag, 1986).

CH 410: CHEMICAL DYNAMICS AND ELECTROCHEMISTRY **L 3 T 0 P 0 CR 3**

Course outcomes:

After completion of the course, the learner shall be able to understand:

CO1: Chemical kinetics of simple and complex reactions

CO2: Analysis techniques for fast reactions

CO3: Kinetics of reactions in solution phase

CO4: Chemistry of ions in solution

CO5: Electrode-electrolyte interface and different electrochemical processes.

Course Content:

Unit 1 **[15 Lectures]**

Brief review of chemical kinetics: Determinations of reaction rates; Kinetics and mechanism; Steady state kinetics, Kinetic and thermodynamic control of reactions, Composite reactions, chain reactions, Oscillatory reactions.

Photophysical and photochemical processes; Fast reactions; study of fast reactions by flow method, relaxation method, flash photolysis, T and P jump and nuclear magnetic resonance method, Femto-chemistry.

Reactions in solutions, Ionic reactions, kinetic salt effect, Electron transfer and proton transfer reactions, Kinetics of enzyme catalysis and micellar catalysis, Phase transfer catalysis, Kinetics and techniques of polymerization, Polymer molecular weight control.

Unit 2 **[5 Lectures]**

Theories of reaction rates: Arrhenius theory, Collision theory, Activated complex theory, Treatment of unimolecular reactions, Lindemann-Hinshelwood, RRK, Marcus and RRKM theory.

Unit 3 **[8 Lectures]**

Equilibrium electrochemistry of ions, hydration number, activity coefficient, Debye-Hückel theory, Debye-Hückel-Onsager treatment and its extension, ion-solvent interactions, Debye-Hückel-Jerum model, electro-capillarity, ion transport, ion channels, Diffusion of ions and molecules in solutions.

Unit 4 **[8 Lectures]**

Electrodes and electrochemical cells, hydrogen electrode, cell reactions, Nernst equation, electrode kinetics, electrode/electrolyte interface, electrical double layer, various models, Exchange current density, Butler-Volmer equation, over potential, Tafel plot, voltammetry, polarography, half-wave potential, Electrocatalysis – influence of various parameters, batteries, solid state battery, fuel cells, electrochemistry of corrosion, anodic/cathodic corrosion and its prevention.

Text Book(s)

1. Atkins, P. and Paula, J. de. *Atkins' Physical Chemistry*, 10^{th} Edn., (Oxford University Press, New Delhi, 2014).
2. Engel, T. and Reid, P. *Thermodynamics, Statistical Thermodynamics and Kinetics*, 2^{nd} Edn., (Pearson, New Delhi, 2011).

Reference book(s)

1. Laidler, K. J. *Chemical Kinetics*, 4^{th} Edn., (McGraw Hill, New Delhi, 2007).
2. Bokris, J. O. M. and Reddy, A. K. N. *Modern Electrochemistry, Vol. I & II*, (Plenum, 2001).
3. Bard, A. J. and Faulkner, L. R. E*lectrochemical Methods: Fundamentals and applications*, 2^{nd} Edn., (Wiley, 2000).

CH 414: QUANTUM CHEMISTRY AND CHEMICAL BONDING-II L 3 T 3 P 0 CR 3

Course outcomes:

After completion of the course, the learner shall be able to learn:

CO1: Born Oppenheimer approximation

CO2: Hartree-Fock method for the solution of Schrodinger equation for many particle system

CO3: Models of chemical bonding-Molecular orbital (MO) and Valence bond (VB) theory

CO4: Hückel π-electron theory and Walsh diagram

Course Content:

Unit 1 **[16 Lectures]**

Born-Oppenheimer approximation, Hartree-Fock method, Brillouin theorem, Koopman's theorem, Roothan's equations, models of chemical bonding - Molecular orbital (MO) and Valence bond (VB) theories, application to diatomic molecules such as, H_2, H_2^+, N_2, O_2, and CO. Hybridisation and MOs of H_2O, NH_3 and CH_4, Introduction to the SCF method.

Unit 2 **[20 Lectures]**

Quantitative MO theory - Huckel π-electron theory and its application to ethylene, butadiene and benzene, energy levels of di- and tri- atomic molecules, Walsh diagrams and molecular geometry, Extended Hückel MO theory and calculation on some simple molecules.

Text Book(s)

1. Atkins, P. W., Friedman, R. S., *Molecular Quantum Mechanics*, (Oxford University Press, 1997).
2. Levine, I. N *Quantum Chemistry*, (Pearson Education, 2004).

Reference Book(s)

1. McQuarrie, D. A. *Quantum Chemistry* (Viva Books Private Limited, 2003).
2. Prasad, R. K. *Quantum Chemistry* (New Age, 2010).

CH 418: ORGANIC REACTIONS AND MECHANISM **L 3 T 0 P 0 CR 3**

Course Outcomes:

On completion of the course, the the learner shall be able to understand:
CO1: Uses of various types of oxidants, reducing agents, selective organometallic reagents in organic synthesis.

CO2: Generation of reaction intermediates and their reaction pathways.

CO3: Important name reactions and molecular rearrangement reactions.

CO4: Pericyclic reactions, photochemical reactions and concept of retrosynthetic analysis.

Course Content:

Unit 1 **[5 Lectures]**

Reduction: Catalytic hydrogenation and dehydrogenation, dissolving metal reduction, hydride reduction of functional groups, Meerwein-Pondrof-Verley reduction, hydroboration and related reaction, reaction of alkyl borane and tributyltin hydride, Wolff-Kishner reduction, non-metallic reducing agents such as diimide.

Unit 2 **[6 Lectures]**

Oxidation: Oxidation by Cr and Mn compounds; oxidation of alcohol, aldehyde, C=C, C-H bonds, PCC, oxidation with per acids and peroxides: C=C, Sharpless epoxidation, Baeyer-Villiger oxidation. Other types: Prevost and Woodward hydroxylation, cis- and trans-hydroxylation, glycol cleavage reagents; $KMnO_4$, OsO_4, HIO_4, $Pb(OAc)_4$, mercuric acetate, SeO_2 oxidation of allylic C-H bond.

Unit 3 **[5 Lectures]**

Rearrangement reactions: Formation and stability of carbenium ions, carbanions, carbenes, nitrenes, radicals, ylides and arynes. Rearrangement reactions involving carbocation (Wagner-Meerwein, Pinacol-Pinacolone rearrangement), carbenes (Wolff & Arndt- Eistert synthesis), nitrenes (Hoffman, Curtius, Schmidt, Lossen, Beckman), acyl cation, PPA cyclization and Fries rearrangement.

Unit 4 **[4 Lectures]**

Photochemistry: Cis-trans isomerisation, Paterno-Buchi reaction, Norrish type I & II reaction, photoreduction of Ketones, dipimethane rearrangement, photochemistry of arenes, Barton reaction.

Unit 5 **[6 Lectures]**

Pericyclic reactions: Orbital symmetry, selection rules and stereochemistry of electrocyclic reaction, cycloaddition and sigmatropic shift, Cheletropic reactions, Diels-Alder reaction-endo/exo-regioselectivity, effect of Lewis acid on Diels-Alder reaction, Claisen, Cope, Sommelet-Hauser rearrangement, Group transfer reactions-ene reaction; and 1,3-dipolar cycloaddition including ozonolysis and reaction of ketene with alkenes.

Unit 6 **[3 Lectures]**

Free radical reactions: Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, reactivity of the attacking radicals, the effect of solvents on reactivity, allylic halogenation by NBS, oxidation of aldehydes to carboxylic acids, auto-oxidation.

Unit 7 **[4 Lectures]**

Selected organic reaction and reagents: Favörski, Hofmann-Loffler-Freytag, ene, Stork-enamine, Michael addition, Robinson annulation, Mannich, Shapiro, Chichibabin and Witting reaction, Gilman's reagent, DCC, LDA, 1,3–dithiane, Baker's Yeast, Phase-transfer catalysts. Boron: organoboron reagents and reactions; Silicon: Organosilicon compounds and their reactions, organotin compounds and their applications.

Unit 8 **[3 Lectures]**

Retrosynthetic analysis: Synthesis backwards, disconnections, synthons (donor and acceptor), choosing disconnections, functional group interconversion, disconnection approach of alcoholic and keto compound, C–C disconnections, natural reactivity and umpolung.

Text Book(s)

1. Clayden, J., Greeves, N., Warren, S., Wothers, P. *Organic Chemistry*, 2nd Edn., (Oxford University Press, 2012).
2. March, J., Smith, M. B. *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, 6th Edn., (Wiley, 2007).

3. Carey, F. A., Sundberg, R. J. *Advanced Organic Chemistry, Part B: Reactions and Synthesis,* 5th Edn., (Springer, New York, 2007).
4. Caruthers, W., Coldham, I. *Modern Methods of Organic synthesis,* 4th Edn., (Cambridge University Press, 2004).
5. Norman, R. O. C., Coxon, J. M. *Principles of Organic Synthesis*, (Blackie Academic and Professional, 1993).

Reference Book(s)

1. Zweifel, G. S., Nantz, M. H., Somfai, P. *Modern Organic Synthesis: An Introduction*, 2nd Edn., (Wiley, New York, 2017).

CH 412: LABORATORY COURSE IN INORGANIC CHEMISTRY L 0 T O P 6 CR 6

Unit 1

Quantitative estimation involving volumetric (redox and complexometry), gravimetric and spectrophotometric methods of analysis of constituents in three component mixtures, alloys and minerals.

Unit 2

Synthesis and characterization of inorganic compounds, including those involving green synthetic methodology: Characterization includes elemental analysis, studies by IR, electronic spectra, magnetic susceptibility, conductance measurements, cyclic voltammetry. TG, DSC.

Text Book(s)

1. Mendham, J., Denney, R. C., Barnes, J. D., Thomas, M. and Sivasankar, B. *Vogel's Quantitative Chemical Analysis*, 6th Edn., (Pearson Education, 2009).
2. Marr, G., Rockett, B. W. *Practical Inorganic Chemistry*, (Van Nostrand, 1972).

Reference Book(s)

1. Wollins, J. D. *Inorganic Experiments*, 3rd Edn., (VCH, 1994).
2. Parshall, G. W. (Ed. in Chief). *Inorganic Synthesis*, *Vol. 15*, (McGraw Hill, 1974).

CH 416: HISTORY OF CHEMISTRY **L 3 T 0 P O CR 3**

Course outcome:

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

CO1: Develop understanding of various branches of science during different eras in different parts of the world

CO2: Analyze the role played by the science in different eras in the evolution of modern day science

CO3: Ethics in science

Course content:

Unit 1 **[10 Lectures]**

Old traditions of Chemical sciences in various countries

Ancient Technology

Medicine in the ancient times

Ayurvedic Chemistry

Alchemy

India, Islamic & Chinese Alchemy

Metal extraction in the ancient times

Fiber, cloth and dying chemistry in the ancient times

Paper and ink in ancient times

Unit 2 **[8 Lectures]**

Construction materials in the ancient times

The iron pillar of Delhi

Science & Technology in the West

Medieval and Renaissance Medicine

Unit 3 **[8 Lectures]**

Modern traditions and methods

The Chemical Revolution: From Boyle to Dalton

Priestley's discovery of dephlogisticated air

Lavoisier and oxygen

Unit 4 **[10 Lectures]**

Discoveries and Inventions in the context of state of art and impact

Development of chemistry during the industrial revolution

Development of chemistry during World War

Ethics in science

Text Book(s)

1. Brock, W. H. *The Chemical Tree: A History of Chemistry*, W. W. (Norton & Co.: New York, 2000).
2. Bell, M. S. *Lavoisier in the Year One*, (W. W. Norton & Co.: New York, 2005).
3. Tripathi, V. Ed. *Archaeometallurgy in India*, (Cambridge University Press, 1998).

Reference Book(s)

1. Singh, M. V. and Shrivastava, B. B. *Science and technology in ancient India*, (Centrum Press, New Delhi, 2011).
2. *Needham J. Science and Civilization in China: Chemistry and chemical technology*, Volume V (Cambridge University Press, 1956).
3. Chattopadhyay, D. P. *History of Science and technology in Ancient India*, (Firma KLM Kolkata, 1986).
4. Ray, P. C. *History of Chemistry in ancient and medieval India,* (Indian Chemical Society, Kolkata, 1956).

CH 501: BIO-ORGANIC CHEMISTRY **L3 T0 P0 CR 3**

Course outcomes:

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

CO1: Structure, Synthesis, Physical and Chemical properties of amino acids

CO2: Structure and therapeutic applications of proteins, Structure of enzyme, Mechanism of enzyme action

CO3: Details about nucleosides, nucleotides, RNA, and DNA including mutagenesis, codon, anticodon, genetic code, transcription and translation.

CO4: Basics, classification, properties, synthesis and biosynthesis of Terpenoids, Alkaloids and Prostaglandins

CO5: Biosynthesis of Shikimic acid, polyketide, derived natural products

Course Content:

Unit 1 **[6 Lectures]**

Bio-organic chemistry: Structure of amino acids and physical and chemical properties, method of synthesis (including Merrifield synthesis) of peptides and polypeptides, naming of polypeptides chain, amino acid sequence determination (N-terminal and C-terminal), structure of protein (Helical and pleated structure), denaturation of protein, biosynthesis of proteins, therapeutic and diagnostic applications.

Unit 2 **[6 Lectures]**

Structure of purines and pyrimidine bases and their biosynthesis, nucleosides and nucleotides and their nomenclature, structure of RNA and DNA, replication of DNA and mutagenesis, codon, anticodon, t-RNA, structure and genetic code, transcription and translation.

Unit 3 **[6 Lectures]**

Enzymes: Mechanism of enzyme action and models, kinds of reactions catalyzed by enzymes, nomenclature, stereochemical aspects, cofactors, co-enzyme chemistry, structure and function of NADH, FAD, ADP and ATP.

Unit 4 **[5 Lectures]**

Terpenoids: Classification, structure, chemistry and biosynthesis of some important mono, sesqui, di and tri-terpenes. e.g. limonene, carvone or carveol etc..

Unit 5 **[5 Lectures]**

Alkaloids: Characteristic reaction, general methods of degradation, structure and chemistry of some well-known alkaloids, e.g. quinine, cocaine, morphine, heroin.

Unit 6 **[4 Lectures]**

Biosynthetic pathway for Shikimic acid, polyketide derived natural products.

Unit 7 **[4 Lectures]**

Prostaglandins: General structure, classification, biosynthetic pathway, stereoselective synthesis of Prostaglandins E_2 and F_2.

Text Book(s)

1. Finar, I. L. *Organic Chemistry* (Volume 2), 6th Edn. (Pearson Education, 2002).
2. Lehninger, A. L. *Principles of Biochemistry,* (Worth Publishers, 1993).
3. Blackburn, G. M., Gait, M. J., Loakes, D., Williams, D. M. ed., *Nucleic Acids in Chemistry and Biology,* 3rd Edn., (RSC publishing, 2006).

Reference Book(s)

1. Salerini, O. L. *Natural and synthetic organic medicinal compounds,* (C. V. Mosby Co. 1976).
2. Mann, J.; Davidson, R. S.; Hobbs, J. B.; Banthrope, D. V., Harborne, J. B. *Natural Products, their chemistry and biological significance*, (Longmann, Essex., 1994).
3. Norman, R., Coxon, J. M. *Principles of Organic Synthesis*, (Blackie, Academic and Professional, 1997).

CH 525: ORGANOMETALLIC CHEMISTRY **L3 T0 P0 CR 3**

Course outcomes:

On completion of this course the students will be able to understand:

CO1: Organometallic compounds with different type of ligands like π-acids, carbenes, alkyls, allyls etc.

CO2: Structure and bonding analysis of organometallic compounds using the MO theory

CO3: Organometallic compounds of main group elements and their structure and bonding analysis

CO4: Application of organometallic compounds as homogeneous and heterogenous catalysts and their role in industrial revolution

Course Content:

Unit 1 **[8 Lectures]**

π- Acid complexes: MO treatment, Preparation, properties, structures and bonding of metal complexes with CO, N_2, NO, PR_3, AsR_3 as ligands, metal carbonyl hydrides and metal carbonyl clusters. LNCC and HNCC, Compounds with metal-metal multiple bonds.

Unit 2 **[8 Lectures]**

Organometallics: Structure, bonding, synthesis and reactions of metal complexes with alkyls, aryls, alkenes, alkynes and allyls, double and multidecker sandwich complexes.

Unit 3 **[8 Lectures]**

Main Group Organometallics: Structure and bonding involving main group (Li, Be, Zn, Hg, Tl, Si, Sn and related systems) and transition elements (Cu, Ag, Au), metal organyls, isolobal analogy.

Unit 4 **[12 Lectures]**

Homogeneous and heterogeneous catalysis: Oxidative addition and reductive elimination reactions, insertion and extrusion reactions, reactions involving co-ordinated ligands, cyclometallation reactions. Catalytic reactions of alkenes– isomerisation, hydrogenation, carbonylation, hydroformylation and polymerization, Fischer-Tropsch process, hydroboration, hydrosilation, hydrocynation, hydroamination.

Text Book(s)

1. Elschenbroich, C., Salzer, A. *Organometallics – A Concise Introduction,* 2nd Edn., (VCH Publication, 1992).

Reference Book(s)

1. Crabtree, R. H. *The Organometallic Chemistry of the Transition Metals,* 6th Edn., (John Wiley, 2014).
2. Powell, P. *Principles of Organometallic Chemistry,* 2nd Edn., (Chapman, London, 1988).

CH 505: LABORATORY COURSE IN PHYSICAL CHEMISTRY L0 T0 P6 CR 12

Unit 1

Purification of chemicals and calibration of analytical instruments; Error analysis-primary and secondary data, accuracy and precision, averaging of data, types of experimental error, significant figures, estimation and representation of error, and minimization of errors, Handling of basic instruments, e.g., potentiometer, conductivity meter, spectrophotometer, etc., through three basic experiments.

Unit 2

Four minor experiments chosen from: Kinetics by spectrophotometry, polarimetry and conductometry, Relative strength of two acids by conductance, Interfacial tension between two liquids by Tensiometer, Determination of a weak acid and a strong acid in mixture by potentiometry, Study of liquid-liquid phase diagram, Determination of fluoride by ion selective electrode, nitrate spectrophotometry, Determination of average molecular weight of a polymer by viscometry, etc.

Unit 3

Four major experiments chosen from: Study of non-Newtonian polymer solutions by Brookfield viscometer, Study of excess adiabatic compressibility of binary system by ultrasonic interferometry, Simultaneous determination of CMC and partition equilibrium constant by spectroscopic method, Kinetics of the catalytic decomposition of H_2O_2 by manganese (IV) oxide, Determination of CMC by Du Nouy Tensiometry, Micellar catalysis by spectroscopy, Determination of pK_a by spectroscopy, Determination of stoichiometry and the stability constant of the complex formation, Study of pseudo-ternary phase diagram of oil-water-(surfactant-cosurfactant) system, Determination of activation energy of reaction by polarometry, Preparation and characterization of nanoparticles etc.

Text Book(s)

1. Viswanathan, B., Raghavan, P. S. *Practical Physical Chemistry*, (Viva Books Pvt. Ltd., 2005).
2. James, A. M., Prichard, F. E. *Practical Physical Chemistry*, 3rd Edn., (Longman, 1974).

Reference Book(s)

1. Jadav, J. B. *Advanced Practical Physical Chemistry*, (Krishna Prakashan, 2015).
2. Garland, G. W., Nibler, J. W., Shoemaker, D. P. *Experiments in Physical Chemistry*, 7th Edn., (McGraw- Hill, 2008).

CH 519: PHYSICAL CHEMISTRY OF SURFACE AND CONDENSED SYSTEMS

L3 T0 P0 CR 3

Course outcomes:

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

CO1: Basic understanding of surface phenomena like curve surface, capillary action, adsorption

CO2: Structure and properties of different colloidal dispersion

CO3: Polymer thermodynamics

CO4: Structure and properties (optical electronic etc.) of solids

CO5: Phenomena occurred on solid surfaces

Course Content:

Unit 1 **[8 Lectures]**

Thermodynamic description of surface and interphase, Surface tension, capillary action, pressure across curved surface, vapor pressure of droplet, Gibbs adsorption isotherm, BET equation, estimation of surface area, Surface film of liquids. Various adsorption isotherms: Freundlich isotherm, Langmuir isotherm, Dubinin-Radushkevich isotherm, Temkin isotherm.

Unit 2 **[8 Lectures]**

Colloids; Surfactants, micelle, thermodynamics of micellization, microemulsion, micellar catalysis. Host-guest chemistry. Lipids and biological membranes, functions of cell membrane, ion transport through cell membrane, nerve conduction, biological cell and its constituents, biomolecules, bioenergetics.

Unit 3 **[6 Lectures]**

Polymer molecular weight determination of polymers and biopolymers, Thermodynamics of polymerization, Thermodynamics of polymer and biopolymer solution, phase separation of polymer solutions, Polymer solution properties, Stereochemistry of polymer.

Unit 4 **[10 Lectures]**

Structures of solids and liquids, liquid crystals, Nanoparticles and nanotechnology, Defects in solids, thermodynamics of Schottky and Frenkel defect formation, Thin films, Langmuir-Blodget film. Electrical properties of solids, intrinsic and extrinsic semiconductors, doping of semiconductors, p-n junction, super conductors, conducting polymers, organic conductors, molecular electronic devices, nonlinear optical materials, optical reflectance, photoconduction, ionic conductors.

Unit 5 [4 Lectures]

Reactions on solid surfaces, Diffusion in solids, Solid state reactions, Solid state batteries.

Zeolites: Synthesis, structure, surface area and catalytic properties; glasses, ceramics and composites.

Text Book(s)

1. Atkins, P. and Paula, J. de. *Atkins' Physical Chemistry*, 10^{th} Edn., (Oxford University Press, New Delhi, 2014).
2. Chakrabarty, D. K. *Solid State Chemistry*, 1^{st} Edn., (New Age Publishers, 2005).
3. Anslyn, E. V. and Dougherty, D. A. *Modern Physical Organic Chemistry*, (University Science Books, 2005).

Reference Book(s)

1. West, A. R. *Solid State Chemistry and its Applications*, 2^{nd} Edn., (Wiley, 2014).
2. Billmeyer, F. W. *Textbook of Polymer Science*, 2^{nd} Edn., (Wiley, 2007).

CH 521: ANALYTICAL METHODS IN CHEMISTRY L3 T0 P0 CR 3

On completion of this course the students will be able to understand:

CO1: Instrumentation technique of various analytical tools like XRD, AAS, cyclic voltammetry, chromatography, optical and electronic microscopy

CO2: Basic principles of those instrumentation techniques

CO3: Application of analytical tools (XRD, SEM, TEM, TGA, AAS, ICP-OES) in characterization and elemental detection of chemical compounds: solids (crystalline, amorphous, nanomaterials), liquids and gases.

CO4: Application of radiochemical techniques in chemical reactions

CO5: Electrochemical techniques for understanding electron transfer reaction mechanism, fuel cell application, Li-ion battery

Course Content:

Unit 1 **[4 Lectures]**

X-ray methods: X-ray diffraction, X-ray fluorescence and X-ray absorption and X-ray emission spectroscopy.

Unit 2 **[4 Lectures]**

Thermoanalytical methods: Thermo gravimetric analysis, differential thermal analysis and differential scanning calorimetry.

Unit 3 **[6 Lectures]**

Electrochemical methods: Coulometry, Polarography, anode-stripping voltammetry, pulse techniques, cyclic voltammetry, electrogravimetry, spectroelectrochemistry.

Unit 4 **[5 Lectures]**

Chromatographic methods: Adsorption, liquid-liquid partition, ion–exchange, paper and thin-layer chromatography, HPLC, gel permeation chromatography and gas chromatography, HPTLC, Flash chromatography.

Unit 5 **[4 Lectures]**

Radiochemical methods: Tracers in chemical analysis, isotopic exchange, isotopic dilution technique, labeling experiments in studying reaction mechanism.

Unit 6 **[8 Lectures]**

Optical microscopy: Optical Rotatory Dispersion and Circular Dichroism: Definition, Deduction of absolute configuration, octane rule for ketones.

Transmission electron microscopy (TEM) and Scanning electron microscopy (SEM).

Unit 7 **[5 Lectures]**

Atomic absorption spectroscopy: Inductively coupled Plasma- mass spectroscopy (ICP-MS), ICP-AES (Atomic Emission Spectroscopy).

Text Book(s)

1. Drago, R. S. *Physical Methods in Chemistry*, (Saunders College, 1992).
2. Hollas, J. M. *Modern Spectroscopy,* (John Wiley, 1996).

Reference Book(s)

1. Willard, H. H. *Instrumental Methods of Analysis*, (East West Press, 1998).
2. Bard, A. J., Faulkner, L. R. *Electrochemical Methods, Fundamentals and Applications,* (John Wiley, 2000).

CH 523: CHEMICAL TECHNOLOGY AND SOCIETY L3 T0 P0 CR 3

Course outcomes:

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

CO1: Basic principles of the techniques generally involved in chemical processing in Industry

CO2: Types of equipment needed in chemical industry

CO3: Exploration of societal and technological issues from a chemical perspective

Course Content:

Unit 1 [20 Lectures]

Chemical Technology: Basic principles of distillation, solvent extraction, solid-liquid leaching and liquid-liquid extraction, separation by absorption and adsorption. An introduction into the scope of different types of equipment needed in chemical technology, including reactors, distillation columns, extruders, pumps, mills, emulgators. Scaling up operations in chemical industry. Introduction to clean technology.

Unit 2 [16 Lectures]

Exploration of societal and technological issues from a chemical perspective. Chemical and scientific literacy as a means to better understand topics like air and water (and the trace materials found in them that are referred to as pollutants), energy from natural sources (i.e. solar and renewable forms), from fossil fuels and from nuclear fission, materials like plastics and polymers and their natural analogues, proteins and nucleic acids, and molecular reactivity and interconversions from simple examples like combustion to complex instances like genetic engineering and the manufacture of drugs. Adverse effects of pesticides, chemical fertiliser, growth hormones and use of aromatic solvents.

Text Book(s)

1. Hill, J. W., McCreary T. W. and Kolb, D. K. *Chemistry for changing times* 13th Edn., (Prentice Hall, 2012)

CH 506: CATALYSIS (PHYSICAL) L3 T0 P0 CR 3

Course outcomes:

On completion of this course the students will be able to understand:

CO1: Various aspects of homogeneous and heterogeneous catalysis

CO2: Catalysts for industrially important reactions like alkene polymerization

CO3: Different spectroscopic and physicochemical techniques for catalyst characterization

CO4: Microporous and Mesoporous materials, their catalytic activity and industrial importance (e.g. in petrochemical industries)

CO5: Reactor design and industrial plant for large scale productions, Future catalysts for environment, biofuels, and energy production

Course Content:

Unit 1 [10 Lectures]

Introduction: Definition, role of catalysts, classification of catalysts. Homogeneous catalysts: Mechanism of homogeneous catalysis, acid-base catalysis, enzyme catalysis, micellar catalysis, phase transfer catalysts, homogeneous catalysis in industry, Ziegler-Natta catalysts, olefin and acetylene polymerization, isomerization, hydrogenation and HY addition, carbonylation reactions, hydroformylation, oxidation of olefins, metallocene catalysts.

Unit 2 **[6 Lectures]**

Theory and mechanism of heterogeneous catalysts: Adsorption and catalysis, mechanism of heterogeneous catalysis, kinetics of heterogeneous catalytic reactions, volcano principle, shape and size selectivity of catalysts.

Unit 3 **[4 Lectures]**

Characterization of catalysts and their surfaces: Methods of surface analysis, surface area, pore size, void fraction, particle size, mechanical strength, surface chemical composition, surface acidity and reactivity.

Unit 4 **[8 Lectures]**

Examples of heterogeneous catalysts: Clays, zeolites, bimetallic, semiconductor and oxide catalysts, supported catalysts, polymer catalysts. Production and design of industrial catalysts: Materials and methods, precipitated catalysts, impregnated catalysts, skeletal catalysts, fused and molten catalysts, calcination, reduction, shape formation of catalyst particles, optimal shape and size of catalysts particle.

Unit 5 **[2 Lectures]**

Reactors: Definition, classification, reactor design, choosing reactors in laboratory and plant.

Unit 6 **[3 Lectures]**

Catalyst promotion and deactivation: Promotion and promoters, causes and mechanism of deactivation, poisoning, sintering, prevention of catalyst decay, regeneration of catalysts.

Unit 7 **[3 Lectures]**

Examples of heterogeneous catalytic reactions: Catalytic processes in petroleum industry- reforming, cracking and hydrotreating, hydrogenation, hydrodesulphurization, Fischer-Tropsch process, etc.

Future Trends: Environmental aspect.

Text Book(s)

1. Bartholomew, C. H., Furrauto, R. J. *Fundamentals of Industrial Catalytic Processes,* 2nd Edn., (Wiley Interscience, 2006).
2. Chakrabarty, D. K., Viswanathan, B. *Heterogeneous Catalysis* (New Age Int., 2008).

Reference Book(s)

1. Gates, B. C. *Catalytic Chemistry*, (John Wiley & Sons, 1992).
2. Wijngaarden, R. J. *Industrial Catalysis,* (Wiley-VCH, 1998).
3. Augustine, R.L. *Heterogeneous Catalysts for Synthetic Chemists,* (Marcel- Dekker, 1996).

CH 508: METHODS IN ORGANIC SYNTHESIS L3 T0 P0 CR 3

Course outcomes:

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

CO1: Enolate chemistry and organometallic reagents

CO2: Important nucleophilc addition reactions, olefination reactions and other name reactions

CO3: Use of umpolung reagents in organic synthesis

CO4: Protection-deprotection chemistry

CO5: Heteroatoms in organic synthesis and retrosynthetic analysis

Course Content:

Unit 1 [8 Lectures]

Alkylation of carbon via enolates and specific enolate equivalents: Generation of carbon nucleophiles by proton abstraction, kinetic vs thermodynamic control in formation of enolates, alkylation of enolates, generation and alkylation of dianions, solvent effect in enolate alkylations, oxygen vs carbon as the site of alkylation, alkylation of aldehydes, esters, lactones and nitro compounds, use of enol derivatives (enamines, vinyl acetates, vinyl-silyl-ethers, C- or O-Sn- derivatives, boron aluminium enolates). Michael addition: 1,2- *vs* 1,4-addition, conjugate addition followed by alkylation, conjugate substitution reactions (Baylis-Hilmann reaction, nucleophilic epoxidation), conjugate addition of organometallic reagents such as Cu-derivatives (Gilman reagents), Grignard reagents, improvements of the Robinson annulation –with alpha –silyl methylvinyl ketone use of vinyl pyridine, Micahel addition of vinyl-silyl-ethers and allylsilanes.

Unit 2 **[6 Lectures]**

Reaction of nucleophilic carbon species with carbonyl groups: Aldol and related condensation reaction, diastereoselective aldol reaction and Michael addition, Mukaiyama aldol reaction, Darzen reaction, Mannich reaction, acylation of nucleophilic carbon, carbonyl olefination (Wittig types reaction and methylenation, recent improvements of the use of phosphorous compounds, ylides, Stereoselective synthesis of alkenes: Julia olefination, Peterson elimination, Wittig reaction, HWE reaction, Still-Gennari modification, Shapiro reaction, McMurry reaction. Metal-mediated alkene synthesis [Tebbe olefination, Petasis reaction, Heck reaction, Suzuki reaction, metathesis (cross metathesis, enyne metathesis, RCM)], stereoselective addition to alkynes (Birch reduction and Lindlar's O_2 reduction).

Unit 3 **[2 lectures]**

Umpolung of reactivity in carbonyl chemistry: Addition of electrophiles to carbonyl carbons, enolate cations (use of ketene thioacetates etc.), homoenolate anions (metalated allyl ethers amines, thio-ethers, silanes), bis-homoenolate cations. Addition reactions of C-C multiple bonds (oxymercuration, hydroboration etc.) and organoboranes.

Unit 4 **[8 Lectures]**

Organometallic compounds in organic synthesis, protective groups (hydroxyl, amine, carbonyl and carboxylic and C-C double bond protecting groups) in organic synthesis. New greener techniques to carry out organic reactions with examples (crown ethers and cryptates, phase transfer catalyzed reaction, micellar catalysis, solid phase synthesis, solvent-free reaction involving mechanical, thermal and microwave energies, use of greener solvents, enzyme catalyzed reaction).

Unit 5 **[6 Lectures]**

Heteroatoms in organic synthesis: Sulfur: Sulfur stabilized anions, sulfonium salts, sulfonium ylides, sulfur stabilized cations, sulfoxides, oxidations using selenium. Important catalyzed reactions such as palladium catalyzed reactions including Heck, Stille, Sonogashira, Kumada, Suzuki & Negishi, alkene metathesis, enyne metathesis, reactions of organoboranes; reactions of organosilicon compounds, reactions of organotin compounds.

Unit 6 **[6 Lectures]**

Retrosynthetic analysis of multistep synthesis, Synthesis: Illustrative synthesis of complex natural products with relevant examples.

Text Book(s)

1. Clayden, J., Greeves, N., Warren, S., Wothers, P. *Organic Chemistry*, 2nd Edn., (Oxford University Press, 2012).
2. March, J., Smith, M. B. *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, 6th Edn., (Wiley, 2007).
3. Carey, F. A., Sundberg, R. J. *Advanced Organic Chemistry, Part B: Reactions and Synthesis,* 5th Edn., (Springer, New York, 2007).
4. Caruthers, W., Coldham, I. *Modern Methods of Organic synthesis,* 4th Edn., (Cambridge University Press, 2004).
5. Norman, R. O. C., Coxon, J. M. *Principles of Organic Synthesis*, (Blackie Academic and Professional, 1993).

Reference Book(s)

1. Zweifel, G. S., Nantz, M. H., Somfai, P. *Modern Organic Synthesis: An Introduction*, 2nd Edn., (Wiley, New York, 2017).
2. Mundy, B. P., Ellerd, M. G. *Name reaction and reagent in organic synthesis,* (John Wiley and Sons. 1998).
3. Smith, M. B. *Organic Synthesis,* 2nd Edn., (McGraw Hill, 2002).

CH 528: SPECIAL TOPICS IN INORGANIC CHEMISTRY L3 T0 P0 CR 3

Course outcomes:

On completion of this course the students will be able to understand:

CO1: Non-covalent force of interactions and supramolecular systems

CO2: MOF, COF and Inorganic host like zeolites for host-guest compounds

CO3: Photochemical reactions involving inorganic complexes and redox active centres

CO4: Photocatalyst for water splitting reactions, semiconductors, Ru-complexes, role of co-catalyst, quencher, quantum yield

CO5: Structure, electronic and bonding properties of unusual organometallic compounds, Computational study of organometallic compounds

Course Content:

Unit 1 [8 Lectures]

Introduction to Supramolecular Chemistry, nature of supramolecular interactions, host design, nanochemistry, host-guest chemistry, supramolecular synthesis of metal-organic and inorganic compounds.

Unit 2 [12 Lectures]

Inorganic Photochemistry: Excited states, ligand field states, charge-transfer states and Thexi states; Phosphorescence and fluorescence; Photochemical reactions: substitution and redox reactions of Cr(III), Ru(II) and Ru(III) complexes, photosystem-I and II, artificial photosynthesis, photocatalytic water splitting, dye sensitized solar cell.

Unit 3 [6 Lectures]

Pi-pi bonding in heavier main group chemistry, concept of Frustrated Lewis Pair (FLP) and their applications, Chemistry of N-heterocyclic carbenes, silylenes and germylenes, Aurophilic interactions.

Unit 4 [10 Lectures]

Theoretical study of the electronic structure of some organometallic compounds.

Text Book(s)

1. Elschenbroich, C., Salzer, A. *Organometallics – A Concise Introduction,* 2^{nd} Edn., (VCH Publication, 1992).
2. Cotton, F. A., Wilkinson, G., Murillo, C. A. and Bochmann, M. *Advanced Inorganic Chemistry*, 6^{th} Edn., (John Wiley, 2007).
3. Ramamurthy, V., Schanze, K. S. *Multimetallic and Macromolecular Inorganic Photochemistry molecular and Supramolecular Photochemistry,* 4^{th} Edn., (Marcel Dekker, 1999).
4. Steed, J.W., Atwood, J. L. *Supramolecular Chemistry*-2^{nd} Edn., (John Wiley Publication, 2009).

Reference Book(s)

1. Crabtree, R. H. *The Organometallic Chemistry of the Transition Metals,* 6^{th} Edn., (John Wiley, 2014).
2. Hammer, F. *Inorganic Photochemistry*, (Sarup Book Publishers, 2009).
3. Porterfield, W. W, *Inorganic Chemistry*, (Elsevier, 1993).

CH 532: Chemistry of Paints and Surface Coating Technology L3 T0 P0 CR3

Course outcomes:

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

CO1.The chemistry behind paints, pigments and surface coating technology

CO2.Industrial processes of making paints

CO3.Chemical modification of vegetable oils

CO4.Basic ideas of polymer blends

Course Content:

Unit I **[6 Lectures]**

Introduction of paints and surface adhesion, classification- paints, varnishes and lacquers, their components and functions, binders, pigments, extenders, and additives, global picture of paint industry.

Unit II **[8 Lectures]**

Chemical modifications of vegetable oils- monoglyceride preparation, thermal polymerization, dehydration of the oil, oxidation, auto oxidations, iodination, hydrolysis, alcoholysis, acidolysis, saponification, sulfonation, epoxidations. Preparation of alkyd resins, acrylic polymers, phenolics, amino resins, epoxy resins, polyurethane resins and polysiloxanes. Curing parameters for all the resins and properties of all the resins.

Unit III **[7 Lectures]**

Pigments: classifications (organic, inorganic pigments), purification and surface modification of pigments, properties of pigments; extenders, fillers and nano fillers; solvents, thinners and diluents, paint additives, physical chemistry of paint formations: wetting, dispersion, stabilization, adsorption, flocculation, rheology; particle size analysis.

Unit IV **[8 Lectures]**

Industrial process for making paints-three roll mill process; ball and pebble mills; sand, bead and short mills, high speed disc dispenser, testing and analysis of paints, general industrial paints, problems of paints and coatings.

Coating Driers: composition, mechanism of drier action; manufacture of driers; evaluation of driers; combination of driers; drier dosage; drier related paint film defects; driers for water based coatings.

Unit V **[7 Lectures]**

Definition and basic concepts of polymer blends, alloys and composites; matrix resins, importance of polymer blends and alloys, principle of polymer miscibility and compatibility, inter-chain forces, interpenetrating network, thermodynamics of polymer miscibility, morphology and phase separation in polymer blends.

Text Books:

1. Swaraj Paul, Surface Coatings: Science and Technology, 2nd Edition, CBS publishers, New Delhi, 2014.
2. Dright G. Welden, Failure Analysis of Paints and Coatings, Wiley, 2009.

3. I.E Nielsen, Mechanical Properties of Polymers and Composites, Vols. 1 & 2, Dekker, New York, 1995

Reference Book:

1. Oil and Colour Chemists' Association, Surface Coating (2 Vols), Tafe Educational Books, Randwick, 1987.

Elective II

CH 514: BIOMOLECULAR CHEMISTRY L3 T0 P0 CR 3

Course outcomes:

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

CO1: Understanding of interface of Chemistry and Biology

CO2: Molecular design of life, biochemical reactions, Chemical and physical foundations of biomolecules

CO3: Detection and isolation of natural biomolecules

CO4: Synthetic and semi synthetic path of biomolecules

Course Content:

Unit 1 [4 Lectures]

Interface of Chemistry and Biology, interaction between drug molecule and receptor sites.

Unit 2 [14 Lectures]

The molecular design of life, biochemical reactions, Chemical and physical foundations of biomolecules : water, acid, base and buffers; the biosynthesis, structure and functions of key biomolecules (nucleic acids, amino acids, peptides and proteins, lipids and carbohydrate); synthesis and oxidations of fatty acids; biological membranes; membrane structure and transport mechanisms, membrane channels and pumps, molecular motors, cell signalling and signal transduction pathways, Principle of thermodynamics; bioenergetics and energy metabolism in cells, carbohydrate and glycobiology, glycolysis and gluconeogenesis, citric acid cycle, oxidative phosphorylation; light reaction of photosynthesis, Calvin cycle.

Unit 3 **[14 Lectures]**

Detection and isolation of natural biomolecules, synthetic and semi-synthetic ways to different biomolecules, stereochemical consequences, protein and DNA X-ray crystallography, biomolecular spectroscopy (absorption and emission spectroscopy, polarization in light scattering, NMR, fluorescence spectroscopy, mass spectrometry for protein identification, vibrational spectroscopy).

Unit 4 **[4 Lectures]**

Biodiversity of natural products

Text Book(s)

1. Blackburn, G. M., Gait, M. J., Loakes, D., Williams, D. M. *Nucleic Acids in Chemistry and Biology,* 3rd Edn*.,* (RSC publishing, 2006).
2. Lehninger, A. L. *Principles of Biochemistry,* (Worth Publishers, 1993).

Reference Book(s)

1. Nogradi, M. *Stereoselective synthesis, A Practical approach,* 2nd Edn*.,* (VCH, Weinheim, 1995).
2. Thomas, G. *Medicinal Chemistry, An Introduction,* (Wiley, 2000, Single Edition).
3. Patrick, G.L. *An Introduction to Medicinal Chemistry,* 2nd Edn*.,* (Oxford University Press, 2001).

CH 516: COMPUTATIONAL CHEMISTRY AND NUMERICAL ANALYSIS L3 T0 P0 CR 3

Course outcomes:

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

CO1: The numerical methods of integration and differentiations

CO2: Molecular mechanics calculation of complex system

CO3: Quantum mechanical calculation of complex systems

Course Content:

Unit 1 **[8 Lectures]**

Data analysis, mean and standard deviation, absolute and relative errors, linear regression, covariance and correlation coefficient. Curve fitting, solution of polynomial equation, numerical integration (Trapezoidal Rule, Simpson's Rule, Gaussian Quadrature), solution of ordinary differential equations (Euler's Method, Runge-Kutta methods, predictor-corrector method), matrix multiplication, inversion and diagonalization.

Unit 2 **[6 Lectures]**

Molecular Mechanics: Basic geometrical description of molecules; force-field development, intermolecular interactions, origin and modelling of dispersion forces & hydrogen bonds, strengths, weaknesses and applicability of currently available force-fields.

Unit 3 **[8 Lectures]**

Static properties of complex systems: Introduction to Monte Carlo as a way of averaging. Metropolis Monte Carlo algorithm: introduction and applications.

Dynamical properties of complex systems: Molecular Dynamics as a way of averaging. Integration of the Newton's equations: initial conditions, numerical algorithms (Verlet and leap-frog), and thermostats.

Unit 4 **[6 Lectures]**

Quantum Chemistry: Many electron systems, Hartree-Fock method, basis sets, electron correlation and its treatment, basics of density functional theory, DFT based reactivity descriptors. Introduction to popular softwares (like Gaussian, DMol, GAMESS). Applications to simple molecular systems.

Unit 5 **[8 Lectures]**

Combined QM/MM methods: Implications of the choice of QM and MM methods; Application of QM/MM methods in organic, inorganic and organometallic systems including bio-organic and bio-inorganic molecules.

Quantitative structure activity relation (QSAR): Early approaches, topological indices, fragmental models; quantum mechanical descriptors.

Text Book(s)

1. Lewars, E. *Computational Chemistry*, (Springer, 2003).
2. Balagurusamy, E. *Numerical Methods,* (Tata McGraw-Hill Publishing Company Limited, 2002).

Reference Book(s)

1. Leach, A. R. *Molecular Modeling: Principles and Applications,* 2nd Edn., (Pearson Prentice Hall, 2001).
2. Cramer, C. J. *Essentials of Computational Chemistry* (Wiley 2002).
3. Jensen, F. *Introduction to Computational Chemistry* (Wiley 1999).

CH 518: ORGANIC SOLID STATES CHEMISTRY **L3 T0 P0 CR 3**

Course outcomes:

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

CO 1: Types of intermolecular interactions

CO 2: Crystal design and crystal design strategies

CO 3: Crystallization techniques of organic solids

CO 4: Concept of polymorphism

CO 5: Understanding of multi-component crystal and coordination polymer

Course content:

Unit 1 **[2 Lectures]**

Intermolecular Interactions: General Properties, van der Waals Interactions, Hydrogen Bonds, Halogen Bonds, Other Interactions.

Unit 2 **[5 Lectures]**

Crystal Engineering: Organic Solid States, Properties, Structure activity Relationship, X-ray Crystallography, Pharmaceutical Developments.

Unit 3 **[5 Lectures]**

Crystal Design Strategies: Synthesis in Chemistry, Supramolecular Chemistry, Synthon in Crystal Engineering.

Unit 4 **[6 Lectures]**

Crystallization of Organic Solids, nucleation, thermodynamics and kinetics of crystallization, crystal growth mechanism, crystal morphology and habit, crystal morphology engineering.

Unit 5 **[6 Lectures]**

Polymorphism: Definition and occurrence, thermodynamic and kinetic relationships of the formation of polymorphs, Methods of polymorph characterization, properties of polymorphs, case studies from the pharmaceutical industry, polymorphism today.

Unit 6 **[6 Lectures]**

Multi-component crystals: classification, definition and nomenclature, solid solutions, Host-Guest compounds, solvates and hydrates, Donor-Acceptor complexes, co-crystals of pharmaceutical importance.

Unit 7 **[6 Lectures]**

Coordination Polymers: Definition, classification and design strategies, network topologies, supramolecular isomerism, interpenetration, porous coordination polymers, properties and applications.

Text Book(s)

1. Desiraju, G. R.; Vittal, J. J.; Ramanan, A. *Crystal Engineering: A Textbook*, (World Scientific Publishing Company, 2011).

2. Bernstein, J. *Polymorphism in Molecular Crystals*, *Monographs on Crystallography*, No. 14, (Clarendon Press/International Union of Crystallography, 2002).

Reference Book(s)

1. Desiraju, G. R. *Crystal Design: Structure and Function*, (John Wiley & Sons, 2003).
2. Steed, J. W.; Atwood, J. L. *Supramolecular Chemistry*, (John Wiley & Sons, 2009).

CH 520: ENVIRONMENTAL AND GREEN CHEMISTRY L3 T0 P0 CR 3

Course outcomes:

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

CO1: Environmental impact and quality parameters of air, water and soil

CO2: Analysis and purification of water, wastewater, solid-wastes and air pollution.

CO3: Environmental protection and pollution prevention

CO4: Green chemistry principles and Design of green synthesis

Course Content:

Unit 1 [6 Lectures]

Environment and chemistry; Matter and cycles of matter; The atmosphere and atmospheric chemistry: The geosphere and geochemistry; Aquatic chemistry, CO_2 distribution, acid-base and redox equilibrium in water, pE-pH curves, water quality parameters.

Unit 2 [6 Lectures]

Chemistry and environmental pollution: Chemical hazards, chemical disasters, Water pollution, air pollution and soil pollution; Industrial pollution, vehicular pollutions, agricultural pollution, pollution by plastics; environmental biochemistry, toxicological chemistry.

Unit 3 [6 Lectures]

Environmental analysis: Analysis of water and wastewater, solid-wastes and air pollution.

Unit 4 **[6 Lectures]**

Environmental protection: pollution prevention, green chemistry, biodegradation, water and wastewater purification – removal of arsenic, iron, fluoride, etc.; air purification, waste minimization, industrial and municipal waste treatment and soil remediation.

Unit 5 **[6 Lectures]**

Green chemistry principles: Principles of green chemistry, atom economy, less hazardous chemical syntheses, designing safer chemicals, safer solvents and auxiliaries, design for energy efficiency, renewable feedstock, catalysis, design for degradation, real time analysis for pollution prevention, and inherently safer chemistry for accident prevention.

Unit 6 **[6 Lectures]**

Design of green synthesis: Ideal synthesis, clean routes, supercritical solvents, ionic liquids, green catalyst, auto-exhaust catalyst and clean technology

Real world examples.

Text Book(s)

1. Manahan, S. E. *Environmental Chemistry*, 9th Edn. (CRC Press, Boca Raton, 2010).
2. Anastas, P. T. and Warner, J. C. *Green Chemistry: Theory and Practice*, (Oxford University Press, 1998).

Reference Book(s)

1. Hutzinger, O. *Handbook of Environmental Chemistry*, (Springer-Verlag, 1991).
2. Cann M. C., Connelly, M. E., *Real World Cases in Green Chemistry*, (ACS, 2000).

CH 534: INDUSTRIAL POLYMERS L3 T0 P0 CR 3

Course outcomes:

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

CO1: Fundamentals of industrial polymers

CO2: Synthesis, processing and properties of some industrially important polymers

CO3: Discussion of the applications of the polymeric products

Course Content:

Unit I **[4 Lectures]**

Fundamentals of industrial polymers including monomer, initiator, catalyst; manufacturing techniques, structure and property, modification, applications, etc.

Unit II **[8 Lectures]**

Industrial commodity thermoplastics like polyethylene, polypropylene, polystyrene, poly(vinyl chloride), high impact polystyrene, etc.; their preparative methods, microstructures, physical, mechanical, thermal, chemical and aging properties; various commodity to advanced applications.

Unit III **[8 Lectures]**

Industrial engineering thermoplastics like poly(acrylonitrile), nylon 6, nylon 6,6, polyesters, polycarbonates, polyurethanes, poly(tetrafluoroethylene), etc. their preparative methods, microstructures, physical, mechanical, thermal, chemical and aging properties; various commodities to advanced applications.

Unit IV **[8 Lectures]**

Industrial thermosetting resins like phenolic resins, amino-resins, alkyds, unsaturated polyesters, polyurethanes, epoxy resins, etc.; their preparative methods, microstructures, physical, mechanical, thermal, chemical and aging properties; various commodity to advanced applications.

Unit V **[8 Lectures]**

Industrial elastomers like natural rubber, styrene-butadiene rubber, acrylonitrile-butadiene rubber, synthetic isoprene rubber, isobutylene-isoprene rubber, chloroprene rubber, ethylene-propylene diene rubber, chlorosulphonated polyethylene rubber, silicone rubber, fluororubbers, etc. their preparative methods, microstructures, physical, mechanical, thermal, chemical and aging properties; various commodity to advanced applications.

Text Books

1. P. Ghosh, Polymer Science and Technology: Plastics, Rubbers, Blends and Composites, Third Edition, McGraw Hill Education Private Limited (India), 2011
2. J. A. Brydson, Plastics Materials, 4th edn., Butterworths, London, 1982
3. J. A. Brydson, Rubbery materials and their compounds, Elsevier Applied Science, London, 1988

Reference Book

1. M. Chanda, S. K. Roy, Industrial Polymers, Specialty Polymers, and Their Applications, 1st Edition, CRC Press, 2019.
2. E. Alfredo Campo, Industrial Polymers, Carl Hanser Verlag GmbH & Co. KG, Berlin, 2007

CH 522: POLYMER CHEMISTRY (PHYSICAL/ POLYMER) L3 T0 P0 CR 3

Course outcomes:

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

CO1: Historical background and basics of polymer chemistry

CO2: Kinetics of polymerization reaction

CO3: Basic characterization of polymers

CO4: Thermodynamics of polymer solutions

CO5: Structure-property relationship of polymers

Course Content:

Unit 1 [3 Lectures]

Introduction: Historical background, basic nature, classification, raw materials for polymers, gas cracker, naphtha cracker.

Unit 2 **[5 Lectures]**

Kinetics and mechanism of polymerization: Degree of polymerization and molecular weight of polymer, kinetics of various types of polymerization, co-polymerization, reactivity ratio, molecular weight distribution, control of molecular weight.

Unit 3 **[3 Lectures]**

Polymerization techniques: Special features of polymerization, various polymerization techniques, polymerization reactors.

Unit 4 **[7 Lectures]**

Polymer characterization: Determination of molecular weight and molecular weight distribution, GPC, light scattering, end group analysis method, Zimm plot, viscosity of polymer solutions, thermal, mechanical, rheological and electrical properties of polymers, polyelectrolytes, ion-exchange resins.

Unit 5 **[7 Lectures]**

Thermodynamics of polymer solutions: Chain conformation, molecular dimensions in solution, solubility of polymers, solubility parameters, lattice theory, ΔH, ΔS and ΔG of mixing in polymer solution, dilute polymer solutions, χ_1 and θ-temperature, phase separation, fractionation.

Unit 6 **[3 Lectures]**

Structure-property relationship: Stereochemistry of polymers, cross-linking, polymer architecture, elasticity, viscoelasticity, crystallinity.

Unit 7 **[8 Lectures]**

Natural polymers: rubber, natural fibers, silk fibers, Synthetic polymers: HDPE, LDPE, PP, PS, Nylon; synthetic polymeric resins and rubbers, moulding, Applications and Future trends: Applications, degradation and future trends

Text Book(s)

1. Misra, G.S. *Introductory Polymer Chemistry* (Wiley Eastern Limited, 1993).
2. Billemeyer, F. *Textbook of Polymer Science* (Wiley, 1984).

Reference Book(s)

1. Odian, G. *Principles of Polymerization* (Wiley, 2004).
2. Sun, S. F. *Physical Chemistry of Macromolecules,* 2^{nd} Edn*.,* (Wiley, 2004).
3. Seymour, R. B. *Polymer Chemistry: An Introduction* (Marcel-Dekker, 1984).

CH 524: HETEROCYCLIC COMPOUNDS AND MEDICINAL APPLICATIONS (ORGANIC)

L3 T0 P0 CR 3

Course outcomes:

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

CO1: Modern approaches to drug design and clinical trials

CO2: Importance of heterocyclic compounds in medicinal chemistry and drug design

CO3: Nomenclature, classification, synthesis and reactivity of non-aromatic, aromatic, benzo-fused heterocycles containing one, two or more heteroatom

Course Content

Unit 1 **[6 Lectures]**

History of medicinal chemistry, interaction between drug molecule and receptor sites, drug action mechanism, drug metabolism, approaches to drug design; pharmacokinetics-pharmacodynamics, xenobiotics. Drug development, screening, lead optimisation, phase I, II and III trials.

Unit 2 **[4 Lectures]**

Introduction to heterocyclic compounds: Nomenclature, classification, heterocycles and aromaticity, importance of heterocycles in medicinal chemistry.

Unit 3 **[7 Lectures]**

Non-aromatic heterocycles: Syntheses and reactivities of small ring non-aromatic strained heterocycles like epoxides, aziridines, azetidines, oxetanes, thietanes.

Syntheses, conformations and medicinal importance of six-membered non-aromatic heterocycles like piperdines, piperzines, morpholines, tetrahydropyrans.

Unit 4 **[7 Lectures]**

Benzo-fused heterocycles containing one heteroatom: Syntheses and reactions of benzo-fused heterocycles containing one heteroatom *e.g*. benzofurans, 2,3-dihydrobenzofurans, benzothiophenes, benzopyrans, 1,2,3,4-tetrahydroquinolines etc. Examples and selected syntheses of some important drugs containing this class of benzo-fused heterocycles.

Unit 5 **[6 Lectures]**

Aromatic heterocyclic compounds containing one hetero atom: Preparation and properties of furan, thiophene, pyrrole, indole, quinoline and isoquinoline derivatives.

Unit 6 **[6 Lectures]**

Heterocyclic compounds containing two or more hetero atoms: Synthetic methods of preparation, properties and applications in medicinal chemistry ~~e.g.~~, azoles (pyrazole, imidazole, oxazole and thiazole derivatives), diazines (pyrazine, pyrimidine and pyridazine derivatives), benzo-diazines, heterocyclic compounds containing one nitrogen atom and an oxygen or sulphur atom (oxazine, phenoxazine and thiazine derivatives), triazines and tetrazines.

Text Book(s)

1. Abraham, D. J. ed., *Burger's Medicinal Chemistry and Drug Discovery (6 volume set),* 6^{th} Edn*.,* (Wiley Interscience, 2003).
2. Thomas, G. *Medicinal Chemistry, An Introduction,* (Wiley, 2000, Single Edition).
3. Finar, I. L. *Organic Chemistry* (Volumes I and II), 6^{th} Edn., (Pearson Education, 2002).
4. Joule, J. A., Mills, K. *Heterocyclic Chemistry*, 5^{th} Edn., (Wiley, New York, 2010).

Reference Book(s)

1. Gilchrist, T. L. *Heterocyclic Chemistry*, 3^{rd} Edn., (Pearson India, 2008).

2. Patrick, G. L. *An Introduction to Medicinal Chemistry,* 2nd Edn., (Oxford University Press, 2001).

CH 526: BIO-INORGANIC CHEMISTRY (INORGANIC) L3 T0 P0 CR 3

Course outcomes:

On completion of this course the students will be able to understand:

CO1: .Biological importance of calcium, Na and K

CO2: Metalloenzymes, non-heme protiens and their biological functions

CO3: Toxicity of metals like mercury, cadmium and lead

CO4: Metal complexes as anticancer drugs

CO5: Application of metals for medical diagnosis

Course Content:

Unit 1 [8 Lectures]

Calcium in biology: Calcium in living cells, transport and regulation, molecular aspects of intramolecular processes, extracellular binding protiens. Role in muscle contraction, blood clotting mechanism and biological calcification. Na-K Pump.

Unit 2 [16 Lectures]

Protiens and enzymes of Fe, Co, Cu, Mo and Zn: Hemerythrin, ferritin and transferrins, peroxidase, catalase, cytochrome P-450. Iron–sulphur proteins: rubredoxin and ferredoxins. Cytochrome C oxidase and superoxide dismutase, ceruloplasmin, Vitamin B12, B12 co-enzymes and cobalamines, carbonic anhydrase, carboxy peptidase, metallothionins, interchangeability of Zn and Co in enzymes. Structural and functional models, Biological nitrogen fixation.

Unit 3 [12 Lectures]

Metals in medicine: Toxicity of mercury, cadmium, lead, chromium, beryllium, selenium and arsenic, biological defence mechanisms, chelation therapy, metals used for diagnosis and chemotherapy, platinum complexes as anticancer drugs, complexes of gold, copper, zinc, mercury, arsenic and antimony as drugs.

Text Book(s)

1. Cowan, J. A. *Inorganic Biochemistry- An Introduction*, (Wiley- VCH, 1997).
2. Hanzlik, R. P. *Inorganic Aspects of Biological and Organic Chemistry*, (Academic Press, 1976).

Reference Book(s)

1. Lippard, S. J., Berg, J. M. *Principles of Bioinorganic Chemistry*, (University Science Book, Mill Valley, 1994).
2. Hay, R. W. *Bioinorganic Chemistry*, (Ellis Hollwood, 1984).

CH 536: CHEMISTRY OF MATERIALS **L3 T0 P0 CR 3**

Course outcomes:

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

CO1: Solid state conductors, both electron and ion conductors, and their structure-property correlation and application

CO2: Polymeric materials (organic and inorganic) and their properties

CO3: Liquid crystals, their characteristic properties and applications

CO4: Clay-polymer and carbon composite

Course Content :

Unit 1 **[8 Lectures]**

Solid state ionic conductors: Structure, physico-chemical principles, applications.

Ferrous alloys, Fe-C phase transformations in ferrous alloys; non-ferrous alloys-properties and applications of ferrous and non-ferrous alloys, magnetic alloy. Metallic glass, ceramics, Nano-materials and optical materials.

Unit 2 **[6 Lectures]**

Polymeric materials: Molecular shape, structure and configuration, crystallinity, stress-strain behaviour, thermal behaviour, polymer types and their applications, conducting and ferro-electric properties.

Unit 3 **[7 Lectures]**

Inorganic Polymers: Polysiloxanes, polysilanes, polyphosphazenes, polymeric sulphur – synthesis, structure, properties and applications. co-ordination polymers and organometallic polymers.

Unit 4 **[7 Lectures]**

Liquid crystals: Nomatic, smectic, cholesteric–properties and applications. High Tc materials: Defect Perovskites- high Tc superconductivity in cuprates, 1-2-3 and 2-1-4 materials; anisotropy, temperature dependence of electrical resistance, optical phonon modes, superconducting state, heat capacity, coherence length, elastic constants, position lifetimes, micro-wave absorption pairing and multigap structure in high Tc materials, applications of high Tc materials.

Unit 5 **[8 Lectures]**

Organic solids: Conducting organics, organic superconductors, Magnetism in organic materials.

Fullerenes: doped fullerenes as superconductors.

Molecular devices: molecular rectifiers and transistors, artificial photosynthetic devices, sensors.

Clay-polymer composite and carbon composites, phosphor and laser materials.

Text Book(s)

1. Keer, H. V. *Principles of the Solid State* (Wiley Eastern, 1993).
2. Ashcroft, N. W. and Mermin, N. D. *Solid State Physics* (Saunders College, 1993).

Reference Book(s)

1. Callister, W. D. *Material Science and Engineering- An Introduction* (Wiley, New York, 1985).
2. Lever, K. D.; Alexender, J. M. and Rawlings, R. D. *Materials Science* (J.C. Senderson, ELBS).
3. Marck, J. E.; Allcock, H. R. and West, R. *Inorganic Polymers* (Prentice Hall, 1992).

The end