Curriculum Structure for 4th year of FYUGP and 1 Year PG Programme
Department of Chemistry, Gauhati University

B. Sc. Semester 7 ***(M. Sc. Semester 1)***				
CourseType	**Course**	**Course code**	**Credit**	**L-T-P***
Core	Inorganic Chemistry 1	CHE070104	4	2-1-1
Core	Organic Chemistry 1	CHE070204	4	2-1-1
Core	Physical Chemistry 1	CHE070304	4	2-1-1
Core	Quantum Chemistry	CHE070404	4	2-1-1
	Research Methodology		4	
B. Sc. Semester 8 ***(M. Sc. Semester 2)***				
Core	Inorganic Chemistry 2	CHE080104	4	2-1-1
Core	Organic Chemistry 2	CHE080204	4	2-1-1
Core	Physical Chemistry 2	CHE080304	4	2-1-1
Core	Spectroscopy	CHE080404	4	2-1-1
Elective	One seminar	CHE080504	4	2-1-1
Elective	**Project** based course **and** presentation	CHE080604	4	0-0-4
1 year PG 1st Semester ***(M. Sc. Semester 3)***				
Core/Elective	Biochemistry	CHE090104	4	2-1-1
Core/Elective	Foundations of Organic synthesis and Green Chemistry	CHE090204	4	2-1-1
Core/Elective	Materials Chemistry	CHE090304	4	2-1-1
Core/Elective	Supramolecular Chemistry	CHE090404	4	2-1-1
Core/Elective	Surface Chemistry and Catalysis	CHE090504	4	2-1-1
Core/Elective	Advanced Bioinorganic Chemistry	CHE090604	4	2-1-1
1 year PG 2nd Semester ***(M. Sc. Semester 4) Research***				
	Project based Dissertation	CHE100101	20	0-0-20
1 year PG 2nd Semester ***(M. Sc. Semester 4) Coursework***				
Core/Elective	Environmental Chemistry	CHE100204	4	2-1-1
Core/Elective	Advanced Physical Chemistry	CHE100304	4	2-1-1
Core/Elective	NMR Methods for Structure Elucidation	CHE100404	4	2-1-1
Core/Elective	Advanced Organic Synthesis	CHE100504	4	2-1-1
Core/Elective	Natural Products Chemistry	CHE100604	4	2-1-1

Core/Elective	Medicinal Chemistry	CHE100704	4	2-1-1

*** L=Number of *Lecture* classes per week, T= Number of *Tutorials* classes per week, P= Number of *Practical* (laboratory) classes per week.**

Program Specific Outcomes (PSOs)

PSO1. Demonstrate the advanced understanding of chemical substances in terms of functionality, reactivity, selectivity and hazard
PSO2. Operate standard analytical and computational equipments to generate and evaluate experimental and computational data
PSO3. Apply critical thinking and analytical skills to assess and solve real life problems related to chemistry, chemicals and environment
PSO4. Design and develop strategies for creating new methodologies and materials

Semester: 1
CHE070104: Inorganic Chemistry 1
Credits:4
L2-T1-P1

Course Outcomes (COs)

CO1. Explain the fundamentals of group formation.

CO2. Classify molecules on the basis of their symmetry.

CO3. Develop molecular orbitals for complexes.

CO4. Explain bonding in coordination compounds.

CO5. Analyze magnetic properties of inorganic compounds.

Theory (45 Hours)

Unit 1. Molecular Symmetry and the Symmetry Groups (4h)

- Symmetry elements and operations
- Classes of symmetry operations, symmetry and chirality
- Symmetry point groups

Unit 2. 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

Unit 3. Chemical Applications of Group Theory (13 h)

- Group Theory and Quantum Mechanics - wave functions as bases for irreducible representations,
- Direct product and its importance in predicting spectral transition probabilities.
- Symmetry properties of atomic orbitals
- Molecular orbitals for σ and π bonding in AB_4 and AB_6
- Ligand field states, construction of the correlation diagram for the d^2 configuration in an octahedral environment.

Unit 4. Orbital splitting and electronic Spectra of coordination Compounds (12 h)

- CFT, d-orbital splitting in coordination complexes with different symmetries
- Jahn-Teller distortion, CFSE for d^1 to d^{10} systems and pairing energy
- Low-spin and high-spin complexes
- *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 Orgel diagrams, calculation of Dq, B and C, nephelauxetic ratio.

Unit 5. 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
- Magnetic moment - orbital contribution, quenching of contribution, effect of spin orbit coupling
- Magnetic properties of second and third transition series and lanthanides

Laboratory (30 Hours)

1. Molecular orbital calculations of simple inorganic compounds.

2. Density Functional Theory (DFT) calculations for the analysis of Normal Modes (IR and Raman Vibrations).
3. Preparation of bis(*N*,*N*-disalicylideneethylenediammine) and bis(*N*,*N*-disalicylideneethylenediammine) (μ-aquadicobalt(II)). UV-Vis. and IR Characterization.
4. Preparation of *cis*- and *trans*-bisglycinatocopper(II) complex. UV-Vis. and IR Characterization.
5. Solution phase synthesis of co-ordination compounds e.g. vanadylacetylacetonato, trioxalatometal (III)trihydrates etc. (characterization, properties and applications).
6. Determination of magnetic moments of inorganic complexes by using Gouy balance.
7. Determination of Electronic Spin Configuration via Evans Method (magnetic moment measurement).

Books Recommended:

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
3. J. E. Huheey, E. A. Keiter and R. L. Keiter; Inorganic Chemistry: Principles of Structure and Reactivity, 4th Ed. Pearson Education, 2006.
4. B. N. Figgis, M. A. Hitchman; Ligand Field theory and its Applications, Wiley India, 2010.
5. G. L. Miessler, D Tarr; Inorganic Chemistry. 3rd Ed., Pearson Education, 2004.
6. P. W. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong; Shriver & Atkins 'Inorganic Chemistry, 5th Ed. Oxford University Press, 2010.
7. Fundamental Concepts of Inorganic Chemistry, Vols. 1-7, by A.K. Das and M. Das, CBS Publishers and Distributors, 2015.
8. R. L. Dutta, A. Syamal, Elements of Magnetochemistry, 2nd Ed. Affiliated East-West Press Pvt. Ltd.-New Delhi, 2004.
9. F. E. Mabbs, D. J. Machin, Magnetism and Transition Metal Complexes, Dover Pub. Inc., 2008.
10. Reaction Mechanism in Inorganic Chemistry 2nd Ed. R. R. Jordan Oxford University Press, 1998.
11. F. Basolo, R. G. Pearson, Mechanism of Inorganic Reactions 2nd Ed. Wiley Eastern Pvt. Ltd. 1973.

Semester: VII
CHE070204: Organic Chemistry 1
Credits: 4
L2-T1-P1

Course Outcomes (COs)

CO1. Explain the kinetics and energetics of organic reactions.
CO2. Discuss reaction intermediates in organic reactions.
CO3. Analyze the structure and reactivity of reaction intermediates in organic reactions.
CO4. Classify the organic molecules on the basis their stereochemistry and compare their reactivity.
CO5. Analyse and apply qualitative analysis techniques and separation of organic compounds using chromatographic techniques.

Theory (45 Hours)

Unit 1. Kinetics and Energetics of Reaction Mechanism (13 Hours)

- Transition state 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.

Unit 2. Reaction Mechanisms & Intermediates: Structure & Reactivity I (12 Hours)

- Carbanions: enolates and enamines, Kinetic and thermodynamic enolates, name reactions under carbanion chemistry - Claisen, Dieckmann, Knoevenegal, Stobbe, Darzen, Acyloin condensations, Shapiro reaction, Julia olefination, Henry reaction, Nef reaction, Baylis-Hillman reaction.
- Ylids: Chemistry of phosphorous and sulphur ylids.
- Carbocation: structure and stability of carbocations, classical and non-classical carbocations, neighbouring group participation and Wagner-Meerwein rearrangement.

Unit 3. Reaction Mechanisms &Intermediates: Structure & Reactivity II (10 Hours)

- 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, Tebbe olefination reactions.
- Radicals: Generation of radical intermediates and its addition to alkenes, alkynes (inter & intramolecular) for C-C bond formation and Baldwin's rules.

Unit 4. Stereochemistry (10 Hours)

- 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 prochirality); optical purity and enantiomeric excess; conformation of acyclic organic molecules, cyclohexane and decalins.

Laboratory (30 Hours)

1. Qualitative analysis: Binary mixture analysis (solid-solid/solid-liquid/liquid-liquid)
2. Chromatography experiments:
   (i) Qualitative TLC separation and identification
   (ii) Column chromatographic separation of a mixture of compounds.

Recommended Books

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.
7. B. S. Furniss, A. J. Hannaford, P. W. G. Smith, Vogel's Textbook of Practical Organic Chemistry, Pearson, 2012.
8. V. K. Ahluwalia, S. Dhingra, Comprehensive Practical Organic Chemistry, University Press.

Semester VII:

CHE070304: Physical Chemistry 1

Credits: 4

L2-T1-P1

Course Outcomes (COs)

CO1. Evaluate multicomponent chemical systems by analysing the knowledge of phase equilibria and spectroscopy.
CO2. Examine the principles of chemistry using non-equilibrium and statistical thermodynamics.
CO3. Create hands-on skill development on principles of thermodynamics, spectrophotometry using standard reactions inside laboratory.
CO4. Investigate theoretical chemistry experiments by formulating molecular modelling and computational methods.
CO5. Construct chemical information by selecting relevant experimental procedures and assembling results, considering accuracy, precision, limitations, and sources of error.

Theory (45 Hours)

Unit 1. Phase Equilibria and Non-equilibrium Thermodynamics (10 Hours)

- 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: flux, forced flows and entropy of production, coupled flows and phenomenological relations, Onsager reciprocal relations, thermodynamic effects – Seebeck, Peltier and Thomson effect, BZ reaction.

Unit 2. Statistical Thermodynamics (18 Hours)

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

Unit 3. Elementary Spectroscopy (14 Hours)

- 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.

- 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.

Unit 4. Data Analysis (3 Hours)

- Linear Regression and Curve Fitting Techniques

Laboratory (30 Hours): (Minimum of 6 and at least two from each section)

A. **On Spectroscopy**:

1. Determination of the concentration of chromium and manganese in a mixture of dichromate and permanganate by spectrophotometric method.
2. Determination of the composition of iron-salicylic acid complex spectrophotometrically by Job's method of continuous variation.
3. Investigation of the complex ion formation between $Ni^{2+}$and o-phenanthroline by Job's method.
4. Verify the mixture law of refraction and draw the calibration curve for mixtures like glycerol water, n-heptane/n-hexane and hence determine the composition of an unknown mixture of two components.
5. Calorimetric investigation of the reaction between acetone and iodine.
6. Calorimetric determination of the enthalpy of a solution of NH_4Cl from heat capacity.
7. Study of the complex formation between Cu^{2+} ion and ammonia by distribution method and find the composition of the complex.

*Other experiments on spectroscopy can be introduced from time to time

B. **On Thermodynamics**

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 or other adsorbents and estimate the free energy.
3. Determination of thermodynamic quantities ΔH, ΔS and ΔG of dye adsorption on activated carbon.
4. Simulation of real gas using any programming language/computer interface and evaluating the free energy.
5. Determination of the composition of an unknown mixture of two/three components and create a phase diagram.

6. Determination of the equilibrium constant and free energy of the reaction: $KI+I_2 \leftrightharpoons KI_3$ by distribution method.
7. Determination of the molecular surface energy and the association factor for ethyl alcohol.

* Other experiments on phase equilibria/thermodynamics can be introduced as per convenience.

Recommended Books

1. P. Atkins, J. Paula, Physical Chemistry, 12th Edition, Oxford University Press, Oxford 2022.
2. D.A. McQuarrie, J.D. Simon, Physical Chemistry: A Molecular Approach, Viva Student Edition, 1st Edition, 2011.
3. R.S. Berry, S.A. Rice and J. Ross, Physical Chemistry, 2nd Edition, Oxford University Press, Oxford 2007.
4. D.A. McQuarrie, Statistical Mechanics, University Science Books, California, 2008.
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. R.S. Drago, Physical Methods in Chemistry, 1992
7. B. Valuer, Molecular Fluorescence, Wiley-VCH, 2002
8. J.R. Lakowicz, Principles of Fluorescence Spectroscopy, Springer, 3rd Edition, 2006
9. Banwell and McCash, Fundamentals of Molecular Spectroscopy, 4th Edition, McGraw Hill, 2017
10. J.B.Y adav, Advanced Practical Physical Chemistry, Goel Publishing House, 27th Edition, 2008.
11. J.N. Gurtu and A. Gurtu, Advanced Physical Chemistry Experiments, Pragati Prakashan, 6th Edition, 2014.
12. M. Halperin, Experimental Physical Chemistry, 2nd Edition, Prentice Hall, Upper Saddle River, NJ07458
13. Other Sources: *Journal of Chemical Education*, ACS Publications

Semester: VII

CHE070404: Quantum Chemistry

Credits:4

L2-T1-P1

Course Outcomes (COs)

1.Description of Wavepackets and Operators

2.Solving Eigenvalue Equations

3.Execution of Approximate Methods

4.Develop Knowledge of Quantum Mechanics in Simple Systems

5.Execute Mathematical Formulae in Real Molecules

Theory (45 Hours)

Unit 1. Wavepackets and Operators (8 h)

- Eigen values and Eigen vectors, Dirac bra-ket notation, review of vectors and vector spaces, Hilbert space
- Wave equation and interpretation in quantum mechanics, separation of time and space
- variables of the Schrodinger equation, Hermitian operators, matrix elements, The diagonalization of the Hamiltonian, wave-packets, wave functions of one particle and many particles system.
- Born interpretation, expectation values of observable properties.

Unit 2. Solution of Eigenvalue Equations (14 h)

- Solutions of the energy eigenvalue equations for particles in a ring, Rigid Rotor, Angular momentum operators, Step-up and Step-down operators, QM treatment of H-atom and H_2^+ molecule, Wave function of simple atomic and molecular orbitals.
- QM treatment of Harmonic Oscillator, Ladder operators. Free electron MO theory of benzene.

Unit 3. Approximate Methods (13 h)

- HMO treatment for unsaturated carboncompounds, extended Hückel Theory, elements of band theory.
- 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.

Unit 4. Advanced Quantum Mechanics in Atomic Systems (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), L-S and J-J coupling.

Laboratory (30 Hours):

1. Use ball-and-stick models to visualize molecular structures and discuss concepts like bond lengths, angles, and molecular geometry.
2. Using computational software, analyze the molecular orbitals of various molecules to understand their electronic structure and bonding.
3. Least squares fitting and plotting linear and exponential graphs using computer.
4. Plotting the wave function and the energy expressions for particle in a box for n=1,2 and 3 using any spreadsheet software such as MSExcel/Libre Office etc or simple programming language. (GWBasic/ FORTRAN/ python etc).
5. Plotting simple one-dimensional intermolecular potential energies (eg.harmonic, anharmonic, Lennard-Jones potential etc) using any spreadsheet software such as MSExcel/LibreOffice etc or simple programming language (GWBasic, FORTRAN, python etc) and provide necessary interpretation.

6. Geometry optimization (energy minimization) any polyatomic molecules: Making input file through selection of simple calculation method (e.g., Hartree Fock or Density Functional Theory), STO/GTO, basis set using any quantum chemistry software.
7. Perform geometry optimizations (energy minimizations) to calculate the energy of various conformations of molecules (e. g. butane) and predict the most stable conformation.

Recommended Books

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.
5. Quantum Chemistry by Donald A McQuarrie

Semester: VIII
CHE080104: Inorganic Chemistry 2
Credits: 4
L2-T1-P1

Course Outcomes (COs)

CO1. Assess the chemistry of main group elements.
CO2. Summarize the structure, bonding and reactivity of heavy transition metals.
CO3. Explain the structure, bonding and properties of solid state materials.
CO4. Analyze the structure, bonding and reactivity of organometallic compounds.
CO5. Evaluate the mechanisms of inorganic reactions.

Theory (45 Hours)

Unit 1. Descriptive Inorganic Chemistry (16 Hours)

- 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. The hydroboration reaction, organoboranes, tetrahydridoborates – synthesis and synthetic use.
- Compounds of Al, Ga, In and Tl.
- Fullerenes and fullerides; Silica, silicates, clays and zeolites.
- Compounds of Si, Ge, Sn and Pb.
- Phosphates and phosphazenes; sulfur-nitrogen compounds; metal-oxo compounds; metal chalcogenides.
- Organometallic compounds of Li, Be and Mg.
- Chemistry of the second and third transition series elements –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.

Unit 2. Introduction to Solid State Chemistry (6 Hours)

- Structure of simple solids–metals, alloys and compounds; common structure types.
- Bonding in solids–free-electron and band theory of solids.
- Properties of solids– optical, magnetic and electrical properties of solids.

Unit 3. Organometallic Chemistry (15 Hours)

- 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, structure and reactivity of metal alkyls, alkenes, alkynes, arene and carbene complexes; metallocenes.
- Fundamental organometallic reactions: oxidative addition, reductive elimination, insertion, β-hydride elimination.
- Catalysis-hydrogenation, hydroformylation, alkene polymerization, olefin metathesis, Suzuki coupling reaction.

Unit 4. Mechanism of Inorganic Reactions (8 Hours)

- Substitution in octahedral and square planar complexes: Conjugate base mechanism, racemisation, stereochemistry, electron transfer reactions - inner sphere and outer sphere mechanism, Marcus theory.

Laboratory (30 Hours)

1. Quantitative analysis (binary mixture, alloy, ore) - Ca-Mg ore, Cu-Zn alloy, Pb-Sn alloy, Ni in an alloy *etc.*
2. Isomerism in coordination compounds: conversion of chloropentammine cobalt(III) chloride to nitro and nitroso isomers; *cis*- and *trans*-dichloro bis(ethylenediamine)cobalt(III) chloride *etc.*
3. Preparation of polyoxometalates, *e.g.* tetrabutylammonium hexamolybdate(VI) and characterization.
4. Quantitative determination of components in food (Fe, Zn, I, Ca, *etc.*)

Recommended Books

1. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann; Advanced Inorganic Chemistry, 6thed. 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, 2ndEd. 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**.
8. J. Mendham, R. C. Denney, J. D. Barnes, M. Thomas, B. Sivasankar, Vogel's Textbook of Quantitative Chemical Analysis, 6th Edition, Pearson, **2009**.
9. G. Svehla, S. Mittal, Vogel's Qualitative Inorganic Analysis, Pearson Education, 7th Edition, **2013**.

Semester: VIII
CHE080204: Organic Chemistry 2
Credits: 4
L2-T1-P1

Course Outcomes (COs)

CO1. Apply fundamental concepts of organic photochemistry.
CO2. Evaluate the diverse reactions of carbonyl compounds and olefins in photochemistry.
CO3. Analyze complex photochemical rearrangement reactions.
CO4. Evaluate oxidation and reduction reactions in organic synthesis.
CO5. Apply principles of pericyclic reactions to predict reactivity and stereochemistry.

Theory (45 Hours)

Unit 1. Organic Photochemistry (10 Hours)

- Photochemistry of carbonyl compounds: α-cleavage, β-cleavage, intramolecular H-abstraction, addition to π-systems, Paterno-Buchi reaction, Photochemistry of enones.
- Photochemistry of olefins – photostereomutation of cis-trans isomers, cycloaddition, photochemistry of conjugated polyenes, photochemistry of vision.
- Photo-rearrangement reactions, di-π-methane rearrangement, Photo-rearrangement of cyclohexadienones, Barton rearrangement; Singlet oxygen photochemistry.
- Photochemistry of aromatic compounds.

Unit 2. Oxidation Reactions (10 Hours)

- Metal based and non-metal based oxidations (Cr, Mn, Ag, Os, Ru, Se), DMSO, hypervalent iodine and TEMPO based reagents.
- Epoxidation with peracids, Baeyer-Villiger oxidation, Prevost reaction and Woodward modification.
- Sharpless asymmetric epoxidation, Sharpless asymmetric dihydroxylation.

Unit 3. Reduction Reactions (10 Hours)

- Catalytic hydrogenation (Pd/Pt/Ni). Wilkinson catalyst, Noyori asymmetric hydrogenation.
- Metal based reductions using Li/Na in liquid ammonia, Birch reduction, McMurry reaction, dehalogenation and deoxygenations.
- Hydride transfer reagents from Group III and Group IV in reductions ($NaBH_4$ triacetoxyborohydride, Luche reduction, $LiAlH_4$, DIBAL-H, Trialkyl silanes and Trialkyl stannane, Meerwein-Pondorff-Verley reduction.
- Stereo/enantio selective reductions (Chiral Boranes).

Unit 4. Pericyclic Reactions (15 Hours)

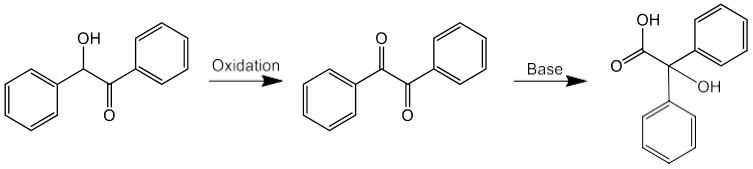
- MO symmetry, FMO of conjugated polyenes. Woodward-Hoffmann principle of conservation of orbital symmetry, allowed and forbidden reactions, stereochemistry of pericyclic reactions, orbital symmetry correlation method, PMO method.
- Cycloaddition reactions: 2+2, 4+2, 3+2 and 4+3 dipolar cycloadditions; stereoselectivity of the reactions, regioselectivity of 4+2 cycloaddition reaction.
- Sigmatropic rearrangement: (m+n) sigmatropic rearrangement of hydrogen and chiral alkyl groups; Divinyl cyclopropane rearrangement, fluxional molecules, stereo selectivity in Cope and Claisen rearrangement. Sommelet-Hauser rearrangement.

- Electrocyclic reactions and cyclo reversions: Conrotatory and disrotatory process, Stereoselectivity of the reactions.

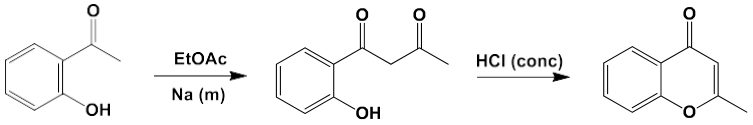
Laboratory (30 Hours)

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

- (Benzoin– Benzil–Benzilic acid): Base catalyzed rearrangement



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



- Oxidation of phenanthrene to phenanthrene-dione and its subsequent condensation to imidazo-phenanthrene derivative.
- Conversion of phthalic anhydride to anthranilic acid via phthalimide.

2. **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).
- Chiral resolution of a racemic mixture by crystallization and determination of enantiomeric excess.

BooksRecommended

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, Oxford University Press 2012.
5. E. V. Anslyn, D. A. Dougherty, Modern Physical Organic Chemistry, University Science Books, 2005.
6. T. H. Lowry, K. S. Richardson, Mechanism and Theory in Organic Chemistry, 3rd Edition, Harper & Row, 1987.

7. B. S. Furniss, A. J. Hannaford, P. W. G. Smith, Vogel's Text book of Practical Organic Chemistry, Pearson, 2012.
8. V. K. Ahluwalia, S. Dhingra, Comprehensive Practical Organic Chemistry, University Press.
9. F. G. Mann, B. C. Saunders, Practical Organic Chemistry, 3rd Edition, Longman, 1978.
10. Selected articles from Journal of Chemical Education, ACS Publications.

Semester: VIII

CHE080304: Physical Chemistry 2

Credits: 4

L2-T1-P1

Course Outcomes (COs)

CO1. Demonstrate the application of chemical kinetics principles

CO2. Analyze molecular reaction dynamics

CO3. Evaluate methods for studying fast reactions

CO4. Critically assess theories of unimolecular reactions

CO5. Apply principles of dynamic electrochemistry

Theory (45 Hours)

Unit 1. Chemical Kinetics (6 h)

- Oscillating reactions, chemical chaos, Belousov-Zhabotinski reaction, branching-chain reactions- the hydrogen-oxygen reaction, explosion limits, enzyme catalyzed reactions, Michaelis-Menten mechanism- Lineweaver-Burk and Eadie plots.

Unit 2. Molecular Reaction Dynamics (6 h)

- The transition state theory (TST) of bimolecular gaseous reactions, statistical and thermodynamic formulations. Comparison between TST and hard sphere collision theory, 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.

Unit 3. Study of Fast Reactions (5 h)

- Stopped flow technique, temperature jump method, relaxation kinetics, linearized rate equation, relaxation time in single step fast reactions, determination of relaxation time.

Unit 4. Theories of Unimolecular Reactions (6 h)

- Theory of unimolecular reactions- Lindemann theory and its limitations, Hinshelwood modification, RRK theory, RRKM theory.

Unit 5. Dynamic Electrochemistry (7 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.

Unit 6. Theories of Electrical Interface (4 h)

- Electrocapillary phenomena- Lippmann equation, electron transfer at interfaces, polarizable and non-polarizable and nonpolaisable interfaces, Butler-Volmer equation, Tafel plot.

Unit 7. Electro-analytical Techniques (6 h)

- Voltametric techniques: cyclic voltammetry, differential pulse voltammetry (DPV), stripping voltammetry techniques
- Potentiometric techniques: ion selective electrodes and other applications
- Amperometric techniques: amperometric sensors and biosensors

Unit 8. Systems for Electro-chemical Energy Storage & Conversion (5 h)

- Batteries: Types of Batteries, Lead-acid batteries, Ni-Cd batteries and Li-ion batteries, Supercapacitors: Electrical double layer capacitor, Pseudo-capacitor, Fuel Cells

Laboratory (30 Hours)

1. Determination of the temperature coefficient and energy of activation of acid hydrolysis of methyl acetate, using leastsquares calculation.
2. Study of the dynamics of an oscillatory reaction.
3. Study of the kinetics of reaction between iodine and acetone in acidic medium by half-life period method anddetermination of the order with respect to iodine and acetone.
4. Study of the decomposition kinetics of the formation of complex between sodium sulphide and sodium nitroprusside spectrophotometrically. Determination of the rate constant and order of the reaction.
5. Study of the kinetics of the reaction between peroxydisulphate and potassium iodide and to find the influence of ionicstrength on the rate constant.
6. Study of the kinetics of oxidation of ethanol by chromium(VI) and to find the rate constant of the reaction. Also find theorder of the reaction by half-life period method.
7. Study of the double exponential time dependence of the reduction of Cr(VI) by glutathione in an aqueous medium andto obtain the rate constants of the process.
8. Determination of the mechanism and rate constant for the oxidation of magnesium by hydrochloric acid.
9. Determination of the relative strength of two acids (HCl and H_2SO_4) by studying the hydrolysis of an ester (methylacetate/ ethyl acetate).
10. Investigation of the inversion of cane sugar in presence of HCl and H_2SO_4 and hence determination of the relativestrengths of the two acids.
11. Investigation of the inversion of cane sugar in presence of acid and hence determination of the activation energy of thereaction.
12. Determination of the equivalent conductivity of acetic acid at infinite dilution by Kohlrausch's method and hence to findthe degree of dissociation constant of the acid.
13. Comparison of the relative strength of acetic acid and monochloroacetic acid by conductance measurement.
14. Determination of the degree of hydrolysis and hydrolysis constant of aniline hydrochloride /sodium acetate.
15. Determination of the strength of the components of the following binary mixture by conductometric titration.
    - Hydrochloric acid and acetic acid
    - Sulphuric acid and copper sulphate
    - Hydrochloric acid and potassium chloride
    - nitric acid and sulphuric acid
16. Determination of the amount of each component of the following ternary mixture by conductometric titration.Hydrochloric acid, acetic acid and copper sulphate
17. Determination of the degree of hydrolysis and hydrolysis constant of CH_3COONa of NH_4Cl by conductance measurement.
18. Determination of the concentration of $AgNO_3$ by conductometric titration against KCl solution.
19. Cyclic voltammetry of a standard solution at different scan rates and calculation of redox potential of electro-active species.
20. Determination of diffusion coefficient from cyclic voltammetry.
21. Determination of Electrode surface area from cyclic voltammetry.
22. Determination of rate of heterogeneous electron transfer from cyclic voltammetry.
23. Chronocoulometry of a redox dye and determination of amount adsorbed on to the electrode surface.

(Students need to perform a minimum of six experiments: at least three from the chemical kinetics experiments and three from the rest)

Recommended Books

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.
6. J. B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 27th Edition, 2008.

Semester: VIII

CHE080404: Spectroscopy

Credits:4

L2-T1-P1

Course Outcomes (COs)

CO1. Explain the theoretical basis of different spectroscopic techniques.

CO2. Analyse rotational, vibrational and Raman spectra, and data interpretation

CO3. Demonstrable understanding of NMR spectroscopy principles, application of advanced NMR methods to examine dynamic processes.

CO4. Apply the principles of EPR spectroscopy to study organic/inorganic compounds.

CO5. Interpretation of mass spectra to deduce structure of biomolecules and organic/inorganic compounds.

Theory (45 Hours)

Unit 1. Rotational and Vibrational Spectroscopy (14 h)

- Rotational spectroscopy: Rotational spectroscopy of symmetric and asymmetric top molecules.
- Raman spectroscopy: polarizability tensor, Stokes and anti-Stokes lines, Origin of characteristic bands, instrumentation and applications in chemical and biological systems.
- Vibrational spectroscopy: Infrared and Raman spectroscopy of simple inorganic and organic molecules, Normal modes of vibrations, organic functional group identification using IR spectroscopy, analysis of representative spectra of metal complexes with various functional groups; application of isotopic substitution.

Unit 2. NMR Spectroscopy (17 h)

- NMR phenomenon, Zeeman splitting, factors affecting sensitivity and resolution of a NMR spectrum, chemical shifttensor,^{1}H NMR-inductive and anisotropic effects on chemical shift (δ), chemical and magnetic equivalence.
- Second order effects in AB, AX and ABX spin systems, simplification of second order spectrum using high magnetic field. Application of ^{13}C NMR (DEPT) and ^{13}Cδ to structural correlations, satellites.
- Pulse and Fourier transformation in NMR in various NMR experiments (1D DEPT and 2D COSY).
- Dynamic processes by VTNMR-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,
- NMR of Si, F, Xe, B, Li and P nuclei. NMR of paramagnetic metal complexes-contact and pseudo-contact shifts; magnetic moment measurement. Introduction to solid-state NMR-CP MAS.

Unit 3. EPR Spectroscopy (8 h)

- Electron Zeeman splitting, g-values, hyperfine and super-hyperfine coupling constants.
- EPR spectra of organic and inorganic radicals/compounds; zero field splitting, Kramer's degeneracy.

Unit 4. Mass Spectrometry (6 h)

- Mass spectrometry: basic principles and instrumentation, 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.

Laboratory (30 Hours)

(Min. 6 experiments are to be performed from the following list of experiments)

1. Interpretation of infrared (IR) spectra of simple organic compounds. (The student is required to learn about identification of functional groups of simple organic compounds by interpreting the IR spectra. The spectra may be recorded and/or provided to the students from literature.)
2. Some representative examples are the following: Group A: eyclohexanol, eyelohexanone, cyclohexane etc. Group B: benzoic acid, salicylic acid, p-cresol etc. The student is required to identify unknowns from group A and B by the process of elimination)
3. Comparison of structural isomers for simple compounds using IR spectroscopy
4. Application of Nuclear Magnetic Resonance (NMR) Spectroscopy for the Characterisation of Small Molecules (e.g. Comparison of trans-2-hexenoic and trans-3-hexenoic acid spectra)
5. Interpretation of EPR spectrum of the simple molecules. (Students will be required to measure the value of g for DPPH and use it to determine the value of g for two inorganic complexes, $Cu(acac)_2$ and $VO(acac)_2$ etc. The spectra will be supplied to the students).
6. Density Functional Theory calculations of Normal Modes and Infrared intensities of simple molecule like water.
7. Structure elucidation of simple molecules using ^{1}H, ^{13}C NMR and mass spectrometry.
8. Interpretation of HR-MS spectrum of one simple organic molecule (The student is required to identify molecular ion peak and base peak; calculate the relative intensities and mass resolutions of all the peaks. The student is also required to propose a fragmentation pattern and explain why measured molecular mass is different from calculated mass. The data file will be supplied to the student).
9. Simulation of the proton NMR spectrum of an AX spin system from density matrices. (The student will be required to simulate the spectrum using density matrices by writing a script).
10. Calculation of chemical shifts of simple organic molecules using GIAO-based method using density functional theory.
11. Analysis of the reduction product of 3-nitrobenzaldehyde and similar compounds using spectroscopic methods.

Recommended Books

1. J. M. Hollas, Modern Spectroscopy, John Wiley & Sons, 4thEd.,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, 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. H. Gunther, NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry, 3rdEdn. Wiley-VCH, 2013.
6. W. Kemp, Organic Spectroscopy, 3rd Edition, Palgrave Macmillan, 2011.

Semester I
CHE090104: Biochemistry
Credits: 4
L2-T1-P1

Course Outcomes (COs)

CO1. Demonstrate understanding of cellular structure and function.
CO2. Analyze bioenergetics and thermodynamics in living systems.
CO3. Evaluate the chemistry of biomolecules.
CO4. Analyze the role of metal ions in biological systems.
CO5. Synthesize knowledge of biochemical principles and apply to real-world scenarios.

Theory (45 Hours)

Unit 1. Introduction (5 Hours)

- 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.

Unit 2. Biophysical chemistry (10 Hours)

- 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.

Unit 3. Bioorganic chemistry (20 Hours)

- 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.
- 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.

Unit 4. Bioinorganic chemistry (10 Hours)

- 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, cytochromes 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.

Laboratory (30 Hours)

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.
- Extraction of DNA from Onion peel.
- Synthesis and characterization of therapeutically relevant metal complexes of first-row transition metals.

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, Bio-inorganic Chemistry; Viva books Pvt. Ltd.1998.
5. J. A. Cowan, Inorganic Biochemistry: An Introduction, 2nd Edition, Wiley,1997.

Semester: IX

CHE090204: Foundations of Organic Synthesis and Green Chemistry

Credits: 4

L2-T1-P1

Course Outcomes (COs)

CO1. Analyze dynamic stereochemistry in organic synthesis.

CO2. Analyze retrosynthetic analysis principles and strategies.

CO3. Evaluate the use of protecting groups in organic synthesis.

CO4. Analyze the synthetic approaches and reactivities of heterocycles.

CO5. Demonstrate synthesis of heterocyclic compounds and apply green synthesis techniques to organic compounds.

Theory (45 Hours)

Part A: Foundations of Organic Synthesis (30 Hours)

Unit 1. Dynamic stereochemistry (8 Hours)

- 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).

Unit 2. Retrosynthetic analysis (7 Hours)

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

Unit 3. Protecting groups (5 Hours)

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

Unit 4. Introduction to heterocycles (10 Hours)

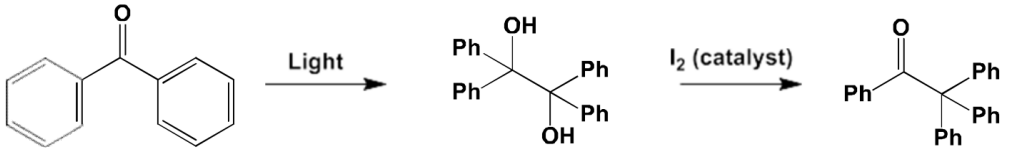
- Synthesis and reactivity of heterocycles containing one heteroatom (O, N, S) including furan, pyrrole, thiophene (Knorr, Paal-Knorr synthesis), pyridine (Hantzsch, Chichibabin synthesis), indole (Fischer, Bischler Synthesis), quinolone and isoquinoline (Combes, Conrad-Limpach, Skraup/Doebner-von Miller, Bischler-Napieralski, Pictet-Gams synthesis).

Part B: Green Chemistry (15 Hours)

- Introductions to green chemistry and its principles (2 Hours)
- Catalysis and green chemistry- water oxidation, conversion of CO_2 utilizing CO_2 as a reactant (5 Hours)
- Renewable raw materials, utilization of renewable biomass, fuels and chemicals from biomass, concepts of platform molecules and conversion of biomass to value-added products (5 Hours)
- Introduction to sustainability, aspects of sustainability ethics, designing sustainable solutions (3 Hours)

Laboratory (30 Hours)

1. Multicomponent reaction of aldehyde, *β*-keto ester and urea/thiourea for the synthesis of dihydro-pyrimidine derivatives (Biginelli reaction).
2. Multicomponent reaction of aldehyde, *β*-keto ester and ammonia for the synthesis of dihydro-pyridine derivatives (Hantzsch Pyridine Synthesis).
3. Benzophenone - Benzopinacol - benzopinacolone): Photochemical, rearrangement.



4. Solvent free reductive amination: Synthesis of imine from aldehyde and amine in solvent free condition and its reduction to amine using $NaBH_4$.
5. Synthesis of an aldol by reacting an aldehyde with a ketone.

Recommended Books

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, 5th Edition, Springer, 2009.
3. M. B. Smith, Organic Synthesis, 2nd Edition, 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.
7. M. Lancaster, Green Chemistry: An Introductory Text, RSC, 2002.
8. P. T. Anastas, J. C. Warner, Green Chemistry: Theory and Practice, Oxford University Press 2008.
9. J. H. Clark, F. Deswarte, Introduction to Chemicals from Biomass, 2nd Edition, Wiley 2015.
10. F. G. Mann, B. C. Saunders, Practical Organic Chemistry, 3rd Edition Longman, 1978.
11. Selected articles from *Journal of Chemical Education*, ACS.

Semester:IX

Paper Code: CHE090304 Materials Chemistry and Nanomaterials

Credits:4

L2-T1-P1

Course Outcomes (COs)

CO1. Describe the fundamental principles of materials chemistry, including the classification of materials based on their chemical composition and structure.

CO2. Apply knowledge of bonding interactions and crystal structures to predict material properties and behaviors in various solid-state systems.

CO3. Synthesize and evaluate the correlation between material structure and properties, specifically in terms of mechanical, electrical, magnetic, optical, thermal, and surface characteristics..

CO4. Analyze data obtained from various characterization techniques such as microscopy, spectroscopy, and diffraction of materials synthesized.

CO5. Evaluate the potential applications of nanomaterials.

Theory (45 Hours)

Unit 1. Introduction to Materials (4 Hours)

- Overview of materials chemistry
- Classification of materials based on chemical composition and structure
- Nanomaterials

Unit 2. Solid state chemistry : (10 Hours)

- Bonding in materials: Ionic, covalent, metallic, and van der waals interactions.
- Crystal structure, crystal symmetry, crystal direction, crystal planes, defects in crystals and their impact on material properties,
- Reciprocal lattice, band structure, density of states and Fermi energy.
- Phenomena in low-dimensional systems- quantum confinement, quantum transport and surface plasmon resonance.

Unit 3: Properties of Materials (6 Hours)

- Structure property correlation Mechanical, Electrical, magnetic, Optical, Thermal and Surface properties of materials in bulk and nanomaterials.

Unit 4: Synthesis Methods (5 Hours)

- Solid-state synthesis techniques, Solution-based synthesis methods, Vapor-phase synthesis techniques, Hydrothermal and solvothermal methods, Nanomaterial synthesis: Bottom-up vs. top-down approaches

Unit 5: Characterization Techniques (8 Hours)

- Optical microscopy and spectroscopy, Scanning electron microscopy (SEM) and transmission electron microscopy (TEM), X-ray diffraction (XRD) analysis, Fourier-transform infrared spectroscopy (FTIR) and Raman spectroscopy, Thermal analysis techniques(DSC, TGA).

Unit 6: Fabrication Techniques (5 Hours)

- Chemical vapor deposition (CVD), Physical vapor deposition (PVD), Electrochemical deposition, Self-assembly and templating methods, Lithography techniques for nanofabrication

Unit 7: Applications (5 Hours)

- Nanoelectronics and nanophotonics, Nanomaterials in energy storage and conversion, Nanomedicine and drug delivery systems, Environmental applications of nanomaterials, Nanomaterials for sensing and diagnostics

Unit 8: Emerging Trends and Future Directions (2 Hours)

- Current trends in materials chemistry and nanomaterials research

Laboratory Experiments (30 Hours)

1. Synthesis of metal nanoparticles by chemical Reduction
2. Characterization of Carbon Nanotubes (CNTs) by Scanning Electron Microscopy (SEM).
3. Fabrication of Thin Film Solar Cells.
4. Preparation and Characterization of Quantum Dots.
5. Electrochemical Deposition of Metal Thin Films.
6. Synthesis of Graphene Oxide (GO) and Reduced Graphene Oxide (rGO).
7. Study of Surface Plasmon Resonance (SPR) in Metal Nanoparticles.
8. Fabrication of Polymer Nanocomposites.

Recommended Books

1. P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong, Shriver & Atkins‘ Inorganic Chemistry, 5th Ed., OUP
2. Bradley D. Fahlman. Materials Chemistry, Springer.
3. A. S. Edelstein; R. C. Cammarata. Nanomaterials: Synthesis, Properties and Applications. CRC Press
4. Charles P. Poole, Frank J. Owens, Introduction to Nanoscience and Nanotechnology. Wiley.
5. Edward L. Wolf. Nanophysics and Nanotechnology: An Introduction to Modern Concepts in Nanoscience. Wiley.
6. Geoffrey A. Ozin; André C. Arsenault. Nanochemistry: A Chemical Approach to Nanomaterials. Royal Society of Chemistry
7. Harry R. Allcock; Frederick W. Lampe; James E. Mark. Introduction to Materials Chemistry. Wiley.
8. A. R. West, Solid State Chemistry and its Applications, Wiley Student Edition, John Wiley & Sons.
9. R. Balasubramaniam, Callister's Materials Science and Engineering, 2nd Edition, Wiley.
10. M.S. Ramachandra Rao, S. Singh, Nanoscience and Nanotechnology: Fundamentals of Frontiers, Wiley India. 2016.
11. G. Schmid, Nanoparticles: From Theory to Application, Wiley-VCH Verlag.
12. G. Cao, Y. Wang, Nanostructures and Nanomaterials Synthesis, Properties, and Applications 2nd Ed. , World Scientific.
13. Gerrard Eddy Jai Poinern, A Laboratory Course in Nanoscience and Nanotechnology, CRC Press.

Semester: IX

CHE090404: Supramolecular Chemistry

Credits: 4

L2-T1-P1

Course Outcomes (COs)

CO1. Describe non-covalent interactions and the concept of pre-organisation in supramolecular chemistry

CO2. Apply knowledge of various supramolecular structures (e.g., crown ethers, cyclodextrins) to understand their applications in molecular recognition.

CO3. Analyze the design, synthesis, and applications of self-assembled structures like metallomacrocycles, MOFs, catenanes, and rotaxanes.

CO4. Evaluate the relevance of supramolecular chemistry in mimicking biological systems, such as using cyclodextrins as enzyme mimics and ion channel mimics.

CO5. Design molecular and supramolecular devices for specific functions, such as photonic devices, electronic devices, and molecular machines.

Theory (45 Hours)

Unit 1. Introduction to Supramolecular Chemistry (7 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.

Unit 2. Synthesis, structure and their applications in recognitions (12 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.

Unit 3. Self-Assembly of molecules (8h)

- 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.

Unit 4. Supramolecular Catalysis (8 h)

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

Unit 5. Molecular Devices (10h)

- Concept 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.

Laboratory (30 Hours)

1. Determination of the CMC of a detergent by surface tension measurement.
2. Preparation and Characterization of a Triple Helicate Complex
3. Synthesis of molecular framework solids
4. Preparation of crown ethers
5. Application of crown ethers as phase transfer catalysts
6. Preparation of a monosubstituted cyclodextrin
7. Preparation of a rotaxane
8. Preparation of a C_{60}-macrocyclic complex
9. Preparation of a Schiff base helicate component

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.
4. P. J. Cragg, A Practical Guide to Supramolecular Chemistry, John Wiley & Sons, 2005.

Semester:V

CHE090504: Surface Chemistry and Catalysis

Credits:4

L2-T1-P1

Course Outcomes (COs)

1. Proficiency in Catalyst Synthesis and Preparation.
2. Demonstration of advanced proficiency in the principles and applications of homogeneous catalysis.
3. Comprehension and application of the properties and functionalities of microporous and mesoporous materials.
4. Proficiency in analysing the operation of catalytic reactors and identifying factors contributing to catalyst deactivation.
5. Analysing Energy-Related Catalysis for insights.

Theory (45 Hours)

Unit 1. Catalysts synthesis and preparation (10 h)

- 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.

Unit 2. Homogeneous Catalysis (10h)

- Atom transfer and electron transfer processes, role of transition metal ions with special reference to 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.

Unit 3. Microporous and mesoporous materials (12 h)

- 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.
- Mesoporous materials - ordered mesoporous materials –synthesis of silica molecular sieve materials - characterization ofmesoporous molecular sieves – catalytic properties of mesoporous materials.

4. Catalytic reactors, deactivation of catalysts (8h)

- Deactivation of catalysts – classification of catalyst deactivation processes; poisoning of catalysts (poisoning of metallic catalysts & poisoning of non-metallic catalysts, poisoning of bifunctional catalysts), metal deposition on catalysts, sintering of catalysts, Regeneration of deactivated catalysts.
- Design of catalytic reactors, Mass flow and heat flow minimisation.

5. Energy and catalysis (5h)

- Energy related catalysis – Perspectives in oil refining – Steam reforming – Water gas shift– Methanol synthesis – CO and CO_2 hydrogenation, Catalytic reforming – Catalytic cracking, Hydrocracking, Catalytic converter, Fuel Cells .

Laboratory:

1. Analyzing the temperature coefficient and energy of activation in the acid-catalyzed hydrolysis of methyl acetate.
2. Study of the autocatalytic reaction between oxalic acid and $KMnO_4$ and determination of the order of the reaction.
3. Determination of the rate constants for the α-chymotrypsin-catalyzed hydrolysis of an ester.
4. Adsorption of dye on activated carbon and analysis of result by different adsorption models.
5. Study of the variation of surface tension of a solution of n-propyl alcohol/ethanol with concentration and determinationof the limiting cross-sectional area of the alcohol molecule.
6. Exploring the base-catalyzed saponification of ethyl acetate with sodium hydroxide, with an aim to determine the reaction order and activation energy.

Recommended Books:

1. G. Ertl, H. Knozinger, J. Weitkamp (Eds), Preparation of Solid Catalysts, Wiley VCH Verlag, 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: IX
CHE090604: Advanced Bioinorganic Chemistry
Credits: 4
L2-T1-P1

Course Outcomes (COs)

CO1. Explain active transport of ions and action potential in nerve impulses.
CO2. Analyze the structural characteristics, functional roles, and catalytic mechanisms of diverse metalloenzymes.
CO3. Evaluate the mechanisms of dioxygen reactions mediated by cytochrome *c* oxidase and oxygenase enzymes, and the role of detoxification enzymes in mitigating oxidative stress.
CO4. Apply principles of electron transport and Marcus theory to analyze electron transport chains in biological system.
CO5. Illustrate relevance of metal complexes in drug design with respect to metal-nucleic acid interactions, photodynamic therapy and diagnostic agents.

Theory (45 Hours)

Unit 1. Metal ion transport (4 Hours)

- Active ion transport across cell membrane, action potential (nerve impulse).

Unit 2. Metalloenzymes (8 Hours)

- Zinc enzymes: Useful characteristics of Zn(II) ion, Metal substitution in Zn enzymes -
- Carbonic anhydrase – structure, function, Co and Cu substitution studies, catalytic mechanism.
- Carboxypeptidase– structure of active site and catalytic mechanism.
- NiFe-hydrogenase, V-peroxidase.

Unit 3. Chemistry of dioxygen (15 Hours)

- Review of NMR and EPR in bioinorganic systems.
- Thermodynamics and kinetics of O_2 reactions -
- Cytochrome *c* oxidase: Spectroscopic characterization and mechanism of dioxygen reduction to H_2O.
- Dioxygenase: Spectroscopic characterization, mechanism and model complex study.
- Monooxygenase: Cytochrome P450 - structure, mechanism, porphyrin based model systems.
- Oxidative stress due to iron and copper *via* Fenton mechanism and its consequences in human diseases; Detoxification enzymes - Catalases, Peroxidases and Superoxide dismutase.

Unit 4. Electron transport systems (8 Hours)

- Iron-Sulfur proteins, Cytochromes , Plastocyanine.
- Electronic coupling matrix, Marcus theory.
- Electron transfer chains– Energy storage and release: Aerobic respiration and photosynthesis; water splitting.

Unit 5. Metal-Nucleic acid interaction (7 Hours)

- Various types of interactions of metal complexes with DNA– coordination, intercalation, insertion, electrostatic and H-bonding and 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 complexes and its therapeutic implications.

Unit 6. Metals in clinical radiology (3 Hours)

- Gd-based MRI contrast agents, ^{99m}Tc and $BaSO_4$ (X-ray contrast agents).

Laboratory (30 Hours)

1. Synthesis and characterization of active site mimics of metalloenzymes:
   (a) zinc enzyme
   (b) catalase, peroxidase
   (c) superoxide dismutase
   (d) oxygenase
   (e) vanadium haloperoxidase, *etc.*

2. Assessment of interaction of metal complexes with DNA (drug-DNA interaction)-
   (a) Determination of intrinsic binding constants (K_b) of metal complexes having flat planar ligands such as phenanthroline bases with calf-thymus (CT)-DNA by UV-visible spectroscopic method.
   (b) Determination of apparent binding constants (K_{app}) of metal complexes by competitive fluorescent displacement method using ethidium bromide.
   (c) Determination of binding affinity of metal complexes with DNA by viscosity measurement.
   (d) Determination of binding affinity of metal complexes with DNA by thermal denaturation method.

3. Assessment of binding affinity of metal complexes with proteins (drug-protein interaction) such as serum albumins (HSA/BSA) by fluorescence quenching method.

4. Assessment of ROS generation (hydroxyl radical, singlet oxygen etc.) abilities of metal complexes spectroscopically (absorption/emission) using chemical probes.

5. Synthesis and characterization MRI contrast agents and their applications.

Recommended Books:

1. Bioinorganic Chemistry by Bertini, Gray, Lippard, Valentine, Viva Books Pvt. Ltd., **1998**.

2. Bioinorganic Chemistry: A Short Course by R. M. Roat-Malone, Wiley Inter science

3. Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life by W. Kaim, B. Schwederski, A. Klein, Wiley 2nd Ed. 2013.

4. Biocoordination Chemistry, D. E. Fenton, Oxford University Press.

5. Biological Inorganic Chemistry: An Introduction, R. R. Crichton, Elsevier.

Semester X

CHE 100204: Environmental Chemistry

Credits: 3 (45 h)

Course Outcomes (COs)

CO1. Analyze the fundamentals and importance of environmental chemistry
CO2. Evaluate the chemistry of the atmosphere and its impact on the environment
CO3. Analyze the environmental chemistry of soil
CO4. Evaluate the environmental chemistry of water
CO5. Synthesize knowledge and apply critical thinking to environmental issues

Theory (45 hours)

1. **Environmental Chemistry: An Introduction (6 h)**
   - Environment & environmental chemistry, Environmental composition, chemical processes, anthropogenic effect and environmental pollution. Role of chemistry in mitigating environmental issues, global concern on climate change, Melting glaciers: causes and effects. Kyoto Protocol, Concept of sustainability and sustainable development, COP27.

2. **Chemistry of the atmosphere (17 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.
   - Stratospheric ozone, ozone formation reactions, ozone destruction reactions, Montreal Protocol, Antarctic and arctic ozone hole.
   - Inorganic air pollutants, control of particulate emissions, Sulphur dioxide & Sulphur cycle, nitrogen oxides in atmosphere, acid rains, energy budget of earth, global warming, carbon footprint, CO_2 sequestration: materials and methods.
   - Organic air pollutants, smog, types of smog, photochemical smog, smog forming reactions of organic compounds, mechanism of smog formation, effects of smog, microplastics in atmosphere.

3. **Soil Environmental Chemistry (10 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 sulphur systems, 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., microplastics, ocean pollution: sources and consequences.

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.

Laboratory (30 hours)

1. Collect water samples from different resources and determine pH, electrical conductivity and Total Dissolved Solids (TDS).
2. Determination of total hardness of water.
3. Determination of total alkalinity and salinity of water.
4. Determination of concentration of metal ions (iron, nickel, chromium, cobalt) present in water using UV-Vis spectrophotometry.
5. Determination of concentration of different organic dyes/pesticides present in water using UV-Vis spectrophotometry.
6. Analysis of acid rain (nitrate, suphate, pH, conductivity and TDS analysis in rain water).
7. Determination of total organic matter present in soil.
8. Adsorptive removal of pollutants (metal ions and organic dyes) present in water using activated charcoal and study kinetics of adsorption.
9. Determination of concentration of humic acid present in soil samples.

Semester IX

CHE100304 **: Advanced Physical Chemistry**

Credits: 4

L2-T1-P1

Course Outcomes (COs)

CO1. Construct atomic and molecular orbitals from mathematical point of view.
CO2. Investigate the physical interplay of light-matter interaction and model subsequent effects on molecular properties.
CO3. Critically analyse the quantum biological aspects of biomolecular systems.
CO4. Design simulated environments of chemical systems using molecular modelling and computational methods.
CO5. Assemble the fundamentals of many-electron theory and create conjectures of complex molecules' properties using approximate methods.

Theory (45 Hours)

Unit 1: Biophysical Chemistry (6 Hours)

- Physical Chemistry of Biomolecules: Stabilizing interactions. Ramachandran Plots and protein structure. Idea of protein folding.
- Ultra-fast biological reactions and conical intersections.
- Drug discovery using Directed Evolution and Artificial Intelligence, AI/ML prediction of molecular properties from spectroscopic and chemical data.

Unit 2. Quantum Dynamics (10 Hours)

- Representation of Atomic and Molecular orbitals in different diagrammatic and algebraic basis vectors. Their time evolution and wave-packet dynamics.
- Idea of Quantum Light: Spontaneous and Stimulated Emission from bonded molecules in Dirac picture and Feynman Diagrams. Dynamics of complex systems.
- Complexities in modelling macromolecular structures and bio-molecules. Potential of mean force and superposition approximation. Quantum Kinetic Equations for energy and particle transport.

Unit 3. Molecular Simulation (7 Hours)

- Molecular Mechanics. Basic geometrical description of molecules: force-fields, intermolecular interactions, origin and modelling of dispersion forces and hydrogen bonds.
- Static properties of complex systems: Introduction to Monte Carlo as a way of averaging. Metropolis, Velocity-Verlet and Leap-frog algorithms: introduction and applications.
- Elements of Quantum Computing.

Unit 4. Many Electron Wave Functions and Operators (10 hours)

- 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.

Unit 5. Approximation Methods (12 Hours)

- 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**.
- Elements of Density Functional Theory.

Laboratory (30 Hours): (Minimum of 6)

1. Computational plotting of atomic and molecular orbitals.
2. Molecule visualization and Quantum Chemical Calculations with GAUSSIAN or GAMESS or Quantum Espresso or DFTB+.
3. Simulation of NMR and IR spectrum of simple molecules with GAUSSIAN or GAMESS or Quantum Espresso or DFTB+.
4. Band structure calculation using GAUSSIAN or GAMESS or Quantum Espresso or any GUI.
5. Simulation of pH metric titration curves, Excel functions LINEST and Least Squares,
6. Numerical curve fitting, linear regression (rate constants from concentration time data) linear regression molar extinction coefficients from absorbance data),
7. Numerical differentiation (e.g. handling data from potentiometric and pH metric titrations, pKa of weak acid),
8. Numerical integration (e.g. entropy/enthalpy change from heat capacity data).
9. Simulation of Ramachandran plots for simple amino acids.
10. d-band center prediction in bimetals using AI.
11. Prediction of pH values from strip colours using AI.
12. Molecular dynamic simulation of a simple protein using any GUI.
13. Experiments on chemoinformatic techniques.
14. Geometry optimization of simple molecules at the HF and DFT levels.
15. Geometry optimization of simple solvated molecules at the HF and DFT **levels**

* Other experiments can be introduced from time to time.

Recommended Books

1. Cantor, C. R. & Schimmel, Biophysical Chemistry, Vol-1-3, W. H. Freeman, 1980.
2. Leach, A. R. Molecular Modelling: Principles and Applications, 2nd Edition, Pearson Prentice Hall, 2001.
3. Cramer, C. J. Essentials of Computational Chemistry, Wiley 2002.
4. Jensen, F. Introduction to Computational Chemistry, Wiley 1999.
5. Landau, L. D. & Lifshiz, I. M., Statistical Physics, Vol-5, Part 1, 3rd Edition, Pegamon Press, 1970.
6. Hill, T. L, Statistical Mechanics: Principles and Selected Applications, Dover, 1987.
7. Mukamel, S, Principles of Nonlinear Spectroscopy, Oxford 1996.
8. A. Szaboo, N. S. Ostlund, Modern Quantum Chemistry, 1st Edition (Revised), 2015.
9. Kauzmann, W, Quantum Chemistry: An Introduction. Academic Press, 1957.
10. Other Sources: *Journal Of Chemical Education*, ACS Publications.

Semester: 3

CHE100404 **~~CHE090804~~: NMR methods for structure elucidation**

Credits:4

L2-T1-P1

Course Outcomes (COs)

CO1. Define key terms used in NMR spectroscopy, such as pulse, chemical shift, coupling constant, dipolar coupling and product operator

CO2. Explain how NMR spectroscopy works and differentiate between various types NMR experiment for chemical shift assignment

CO3. Analyze and interpret 2D NMR spectra to derive molecular structures of organic and natural compounds

CO4. Create simulated NMR spectra for given molecular structures and compare with the experimental outcomes to derive a conclusion

CO5. Critically evaluate the validity of proposed structures based on NMR data in relation to other spectroscopic and chemical information

Theory (45 Hours)

Unit 1. Introductory NMR spectroscopy (10h)

- Isotropic and anisotropic NMR parameters (chemical shifts, *J*-couplings, Nuclear Overhauser effect and dipolar couplings).
- Introduction to pulsed NMR, Product operator analysis for 1D NMR experiment.

Unit 2. 2D NMR experiments and Applications. (15 h)

- Introduction to 2D - NMR.
- Product operator formalism for NMR experiments.
- Perturbative treatment of nonlinear spectroscopic signal.
- Assignment of ^{1}H and ^{13}C chemical shifts by various NMR experiments (^{1}H-NMR, ^{13}C-NMR, COSY, HSQC).

Unit 3. Structure elucidation for organic natural products (13h)

- Determination of constitution, conformation and relative configuration.
- Chemical shift and coupling based DP4 probability methods.
- Determination of absolute configuration using NMR, HR-MS and CD/ORD.
- Molecular modelling using DFT and force fields, geometry optimization, GIOA-based NMR chemical shift calculations and drug-receptor interactions.

Unit 4. Anisotropic NMR for structure elucidation (8h)

- Gel based alignment medium (PMMA).
- Measurement of dipolar couplings. Alignment tensor, Order matrix and *Q*-factor
- Analysis of dipolar couplings for stereochemical determination.

Laboratory (30 Hours)

1. Interpretation of the proton and carbon 1D NMR spectra of simple organic molecules.
2. Assign proton and carbon chemical shifts of simple organic compounds using various NMR experiments (^{1}H-NMR, ^{13}C-NMR, COSY, HSQC).
3. Calculate chemical shifts and *J* couplings using GIAO-based methods using density functional theory.
4. Extract one bond CH *J* couplings from proton-carbon HSQC spectrum of a natural compound and perform *J* based DP4 probability calculations for stereochemistry determination.
5. Extract one bond CH dipolar couplings from proton-carbon HSQC spectrum of a natural compound and perform order matrix analysis for stereochemistry determination.
6. Elucidate the structure of simple organic molecules using HR-MS and NMR data.
7. Perform stereochemical analysis of a chiral compound on the basis of proton and carbon chemical shifts using DP probabilities.
8. Deduce absolute configuration of chiral compounds using CD and NMR.
9. 2D Techniques in the structural elucidation of organic compounds (eg. Cinnamamides).
10. Application of NMR techniques in quality control.
11. Application of NMR methods for the analysis of a sample obtained from natural sources.

Recommended Books:

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 X
CHE100504: Advanced Organic Synthesis
Credits: 4
L2-T1-P1

Course Outcomes (COs)

CO1. Utilize the principles of carbon-carbon bond formation involving Csp^2, and Csp carbon centers, and apply this knowledge in designing synthetic routes.

CO2. Demonstrate asymmetric synthesis techniques, including the use of chiral reagents, catalysts, and auxiliaries, and apply them in the synthesis of enantiomerically pure compounds.

CO3. Demonstrate proficiency in constructing different ring systems, including three, four, five, and six-membered rings, as well as heterocyclic rings, using various synthetic methods.

CO4. Explain synthesis and properties of complex natural products, such as terpenes and alkaloids, applying the principles learned throughout the course.

Theory (45 Hours)

Unit 1a. Synthetic methods (10 Hours)

- Stereocontrolled carbon-carbon bond forming reactions through enolates (including boron and silicon enolates), enamines and silyl enol ethers. Michael addition reaction, Conjugate addition.

Unit 1b. Synthetic methods (7 Hours)

Formation of C-C and C-X bonds involving Csp^2 and Csp carbon centers (with synthetic applications on important namereactions).

Unit 2. Asymmetric Synthetic Methods (10 Hours)

- Enantioselective synthesis (alkylation, allylation and crotylation reactions), use of chiral reagent, chiral catalyst and chiralauxiliary.
- Concepts of asymmetric synthesis: Kinetic resolution.
- Asymmetric Epoxidation (Sharpless, Jacobsen), Asymmetric Dihydroxylation (Sharpless), Asymmetric Reduction (Noyori).

Unit 3. Construction of Ring Systems (10 Hours)

- 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.
- Inter-conversion of ring systems (contraction and expansion); construction of macrocyclic rings, ring closing metathesis.

Unit 4. Synthesis of Complex Molecules (8 Hours)

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

Laboratory (30 Hours)

One-step preparation

I. m-Dinitrobenzene from nitrobenzene.
II. Benzhydrol from benzophenone by reduction in alkaline medium.

III. Beckman rearrangement of cyclohexanone oxime to caprolactam.

Two-step preparation

I. Benzanilide from benzopheone.
II. Benzilic acid from benzoin.
III. Dibenzyl from benzoin.

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, McGraw Hill Higher Education, 2005.
3. R. O. C. Norman, J. M. Coxon, Principles of Organic Synthesis, 3rd Edition, CRC Press.
4. W. Carruthers, I. Coldham, Modern methods of Organic Synthesis, Cambridge University Press, 2005.

Semester: 4

CHE100604: Natural Products and Drug Design

Credits:4

L2-T1-P1

Course Outcomes (COs)

CO1. Define key terms used in natural products and drug design

CO2. To have a comprehensive understanding of natural products, including their sources, chemical structures, and biological activities.

CO2. Explain how drug candidate can be explored from plant based natural products

CO3. Understand various drug design strategies.

CO4. Analyze case studies of successful drug discovery from natural products and explore current trends and applications in the field.

Theory (45 Hours)

Unit1: Introduction to natural products (15 hrs)

- Natural Products: Various sources of natural products, Classification: Types of natural products. Isolation techniques and characterization. Extraction and separation of natural products: nicotin and α-santonin. Structure elucidation of natural products using HR-MS, NMR and CD/ORD. Natural product contributions to human health: morphine and quinine

Unit 2: Essential oil (12 hrs)

- Sources of Essential Oils, Isolation of essential oils (steam distillation method, extraction by means of Volatile solvents), chemistry of essential oils, biological activities of essential oils, industrial uses of essential oils

Unit 3: Drug design (10 hrs)

- Introduction to drug discovery: Sources of drugs-natural products, Drug discovery and development. Drug exploration from plant sources, Identification of hit compound in bio-liquids. Structure based drug design; Fragment based drug design. Polysaccharide vaccine

Unit: Drug-ligand interactions (8 hrs)

- Bing energy-drug potency and selectivity. Drug-receptor interactions: molecular docking, various NMR methods for investigating such interactions.

Laboratory (30 Hours)

1. Extraction of organic compounds from natural sources
   (a) Extraction of nicotine from Tobacco leaves
   (b) Lycopene from tomatoes and β- carotene from carrots.
2. TLC and Paper Chromatography: Separation and identification of the sugars present in the given mixture of glucose, fructose and sucrose by paper chromatography and determination of R_f values.

3. Stereochemical assignment of a natural product by using J couplings and chemical shifts
4. Stereochemical assignment of natural product by using Residual dipolar coupling (RDC)
5. Determination of the molecular properties of caffeine explored by NMR Experiment
6. Calculate the binding energy of a drug-receptor interaction using docking studies
7. Isolation of material from natural sources and its NMR characterization

References

1. Cooper, R.; Nicola, G., *Natural Products Chemistry: Sources, Separations and Structures*; 1st ed.; CRC Press: Boca Ration, **2015.**
2. Santana de Oliveira M.; Almeida da Costa W.; Gomes Silva S. *Essential Oils - Bioactive Compounds, New Perspectives and Application*; 1st ed.; IntechOpen: Rijeka, **2020.**
3. Kumar, R., *Introduction to Drug Designing and Development*. 1st ed.; Nova Science Publishers: USA, **2014.**
4. Fometu, S.; Shittu, S.; Herman, R.; Ayepa, E., Essential Oils and their applications-A mini review. *Advances in Nutrition & Food Science* **2019,** *4*, 1-13.
5. Rudrapal, M.; Egbuna, C., *Computer Aided Drug Design (CADD): From Ligand-based Methods to Structure-Based Aproaches*; Elsevier; **2022**.
6. Keeler, J., *Understanding NMR Spectroscopy*; 2nd ed.; Wiley: Hoboken, **2010.**
7. Haselhorst, T.; Lamberz, A. C.; Itzstein, M., Saturation transfer difference NMR spectroscopy as a technique to investigate protein-carbohydrate interactions in solution. *Methods in molecular biology* **2009**, 534, 375-86.
8. Claridge TDW. Chapter 10 - Diffusion NMR Spectroscopy. In: Claridge TDW, ed. High-Resolution NMR Techniques in Organic Chemistry (Third Edition). Elsevier; **2016**:381-419.
9. Claridge, T. D. W., Chapter 11 - Protein–Ligand Screening by NMR. In High-Resolution NMR Techniques in Organic Chemistry (Third Edition), Claridge, T. D. W., Ed. Elsevier: Boston, **2016**; pp 421-455.

Semester X

CHE100704 Medicinal Chemistry

Credits:4

L2-T1-P1

Course Outcomes (COs)

CO1. Explain basic concepts related to drug action, such as receptors, drug-receptor interactions, and the two-state model of receptor theory

CO2. Apply knowledge of drug discovery and design principles, including the importance of structure-activity relationships (SAR) and molecular modification.

CO3. Analyze the theoretical aspects of drug action, including the factors affecting bioactivity of drugs and the concepts of chemotherapeutic index and therapeutic index.

CO4. Evaluate the importance of various classes of antibiotics, including β-lactam antibiotics, aminoglycosides, tetracyclines, and macrolides, in the treatment of bacterial infections.

CO5. Design strategies for drug discovery and development, including the use of combinatorial libraries and molecular modeling.

Theory (45 Hours)

1. **Introduction & History of Drug Development (4 Hours)**
   - Definition of drug and prodrugs, need of drugs, germ theory of diseases, history of sulpha drugs & their mode of action.

2. **Basic Concepts of Mechanism of Drug Action (5 Hours)**
   - 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 (5 Hours)**
   - Need of quantification of drug action, definition of chemotherapeutic index & therapeutic index, factors affecting bioactivity of drugs, pharmacokinetics and pharmacodynamics, QSAR.

4. **DrugDiscoveryandDesign(5 Hours)**
   - 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 (12 Hours)**
   - Definition of antibiotics, their sources and classification, causes & concerns of bacterial resistance to antibiotics.
   - Natural & semi-synthetic penicillins, SAR and mode of action of penicillin, , bacterial resistance to penicillins - causes and inhibitors, origin of high reactivity of penicillins and related consequences.
   - Aminoglycoside antibiotics (eg.streptomycin, kanamycin), their sources and uses, SAR, mode of action.
   - Teracyclines & chloramphenicol: their therapeutic uses, SAR, mode of action.
   - Macrolideantibiotics: their uses, mode of action, SAR (eg. Erythromycin, azithromycin, telithromycin), peptideantibiotics(toxicityandlimitation).

6. Antimalarials (6 Hours)

- 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 andimportanceindealingwithCQ resistant malaria,modeofaction.

7. Introduction to Viral Diseases &Treatment(4 Hours)

- Difficultyin developingclinicalsolutiontoviraldiseases,introductionto antiviralagents,AIDS– itscauseand prevention

8. Drugs for Treatment of Cancer(4 Hours)

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

Laboratory (30 Hours)

1. Assay of drugs like aspirin, furosemide, Ibuprofen etc.
2. Preparation of drugs/ intermediates like, Benzimidazole, Benzotriazole, Phenytoin etc.
3. Determination of partition coefficient of drugs like ofloxacin, norfloxasin, lomefloxacin etc.

Books Recommended:

1. G.Thomas, MedicinalChemistry:An Introduction,2nd Edition.John Wiley&Sons,2007
2. G.L.Patrick, AnIntroduction toMedicinalChemistry,5th Edition.,OxfordUniversityPress,2013.
3. A.Gringauz,IntroductiontoMedicinalChemistry,WileyIndiaPvtLtd,2010.