PRESIDENCY UNIVERSITY
KOLKATA

04 Years Bachelor Programme under CHOICE BASED CREDIT SYSTME for

B. Sc. Honours with Research in Chemistry

(Total Credits: 194)

Effective from 2023-2024 Academic Session

Aim of the Programme / Programme Outcomes:

1. Create an amicable learning environment among students to inculcate the deep interests and knowledge in subject.

2. Provide choice-based learning to students.

3. Help students to develop the ability to use their knowledge and skills to interpret and handle the problem arises day to day.

4. Motivate students to pursue advanced studies on their subject of interest.

5. Educate and enhancing student generic skills through skill enhancement courses and value added courses, this may help them creating employment and business opportunities in academia and industries.

Programme specific learning outcomes

A graduating student of B.Sc. Chemistry degree expected to:

1. Have proficient theoretical and experimental knowledge in the broad subject area of chemistry as well as different sub-fields of chemistry such as Analytical Chemistry, Inorganic Chemistry, Organic Chemistry, Physical Chemistry, Material Chemistry, etc.
2. Explain, integrate and apply the acquired knowledge to problems that are emerging from the interdisciplinary areas.
3. Be aware of current developments at the forefront in Chemistry and allied subjects.
4. Have hands-on training on various analytical techniques, classical qualitative and quantitative chemical analysis, which creates different types of professionals in the field of chemistry and related fields such as pharmaceuticals, chemical industry, teaching, research, environmental monitoring, product quality, consumer goods industry, food products, cosmetics industry, etc.
5. Have knowledge on hazardous chemical, safe handling of chemicals and role of chemistry on environmental issues.
6. Construct a research problem as per the social requirement.
7. Communicate the scientific work in oral, written and e- formats as per the requirements.

PAPER CODES

8-Semester Bachelor (Hons) programme under CHOICE BASED CREDIT SYSTEM in B. Sc. Honours with Research: 194 Credits (04 Years)

SEM	MAJOR COURSE (C)	AECC	SEC	VAC	MC	MDC
I	CHEM101C01 (Major) CHEM102C02 (Major)	103AECC01	-	-	CHEM104MC01	CHEM105MDC01
II	CHEM151C03 (Major) CHEM152C04 (Major)	153AECC02	-	-	CHEM154MC02	CHEM155MDC02 CHEM156MDC03
III	CHEM201C05 (Major) CHEM202C06 (Major)	-	CHEM241SEC01 (Major)	ENVS204VAC01	CHEM205MC03	-
IV	CHEM251C07 (Major) CHEM252C08 (Major)	-	CHEM291SEC02 (Major)	CHEM292VAC02	CHEM255MC04	-

SEM	MAJOR COURSE (C)	AECC	SEC	VAC	MC	MDC
V	CHEM301C09 (Major)	CHEM341SI01 (Summer Internship)				
	CHEM302C10 (Major)					
	CHEM303C11 (Major)					
VI	CHEM351C12 (Major)	-	-	-	-	-
	CHEM352C13 (Major)					
	CHEM353C14 (Major)					
	CHEM354C15 (Major)					
VII	CHEM401C16 (Major)	-	-	-	CHEM442MC05 (Research Methodology)	-
	CHEM402C17 (Major)					
	CHEM403C18 (Major)					
	CHEM441C19 (Major)					
VIII	CHEM451C20 (Major)	-	-	-	CHEM492MC06 (Research Publication and Ethics)	-
	CHEM452C21 (Major)					
	CHEM453C22 (Major)					
	CHEM491C23 (Major)					

Credit Allocation and Marks Distribution for the 8-Semester Bachelor (Hons) programme under CBCS in B. Sc. Honours with Research, Department of Chemistry, Presidency University, Kolkata

Semester	Course Type	Paper Code	Course Name	Credit			Marks for evaluation		
				Th.	Pr.	Total	Th.	Pr. / CA	Total
I	Major	CHEM101C01	INORGANIC CHEMISTRY-I	4	2	6	70	30	100 (T)
I	Major	CHEM102C02	PHYSICAL CHEMISTRY-I	4	2	6	70	30	100
I	AECC	103AECC01	English Communication /MIL	4		4	100		100 (T)
I	Minor	CHEM104MC01	Atomic Structure, Bonding, General Organic Chemistry, Aliphatic Hydrocarbons	4	2	6	70	30	100 (T)
I	MDC	CHEM105MDC01	Chemistry in Daily Life	3		3	35	15	50 (T)
			Semester-I Total	**19**	**6**	**25**	**345**	**105**	**450**
II	Major	CHEM151C03	INORGANIC CHEMISTRY-II	4	2	6	70	30	100 (T)
II	Major	CHEM152C04	ORGANIC CHEMISTRY-I	4	2	6	70	30	100 (T)
II	AECC	153AECC02	English Communication /MIL	4		4	50		50 (T)
II	Minor	CHEM154MC02	Chemical Energetics, Equilibria & Functional Organic Chemistry	4	2	6	70	30	100 (T)
II	MDC	CHEM155MDC02	Chemistry of Dyes, Colours, Application of Dyes and The Chemistry of Fireworks	3		3	35	15	50 (T)
II	MDC	CHEM156MDC03	Elements of Matter and States of Matters	3		3	35	15	50 (T)
			Semester-II Total	**22**	**6**	**28**	**330**	**120**	**450**
III	Major	CHEM201C05	ORGANIC CHEMISTRY-II	4	2	6	70	30	100 (T)
III	Major	CHEM202C06	PHYSICAL CHEMISTRY-II	4	2	6	70	30	100 (T)
III	SEC (Major)	CHEM241SEC01.1 **OR** CHEM241SEC01.2	IT Skills For Chemists **OR** Quality Control Analysis of Commercial Products	4		4	50		50 (S)
III	VAC	ENVS204VAC01	Environmental Science	3		3	50		50 (T)
III	MC	CHEM205MC03	Solutions, Phase Equilibria, Conductance, Electrochemistry & Functional Group Organic Chemistry	4	2	6	70	30	100 (T)
			Semester-III Total	**19**	**6**	**25**	**310**	**90**	**400**
IV	Major	CHEM251C07	INORGANIC CHEMISTRY-III	4	2	6	70	30	100 (T)
IV	Major	CHEM252C08	PHYSICAL CHEMISTRY-III	4	2	6	70	30	100 (T)
IV	SEC (Major)	CHEM291SEC02.1 **OR** CHEM291SEC02.2	Pharmaceutical Chemistry & Chemistry of Non-covalent Compounds **OR** Green Methods in Chemistry	5		5	50		50 (S)

IV	VAC	CHEM254VAC02	INDUSTRIAL CHEMISTRY	3		3	35	15	50 (T)
IV	MC	CHEM255MC04	TRANSITION METAL & COORDINATION CHEMISTRY, STATES OF MATTER & CHEMICAL KINETICS	4	2	6	70	30	100 (T)
			Semester-IV Total	**20**	**6**	**26**	**295**	**105**	**400**
V	Major	CHEM341SI01	SUMMER INTERNSHIP	4		4	50		50 (S)
V	Major	CHEM301C09	INORGANIC CHEMISTRY-IV	4	2	6	70	30	100 (T)
V	Major	CHEM302C10	ORGANIC CHEMISTRY-III	4	2	6	70	30	100 (T)
V	Major	CHEM303C11	PHYSICAL CHEMISTRY-IV	4	2	6	70	30	100 (T)
			Semester-V Total	**16**	**6**	**22**	**260**	**90**	**350**
VI	Major	CHEM351C12	INORGANIC CHEMISTRY-V	4	2	6	70	30	100 (T)
VI	Major	CHEM352C13	ORGANIC CHEMISTRY-IV	4	2	6	70	30	100 (T)
VI	Major	CHEM353C14	PHYSICAL CHEMISTRY-V	4	2	6	70	30	100 (T)
VI	Major	CHEM354C15	ORGANIC CHEMISTRY-V	4	2	6	70	30	100 (T)
			Semester-VI Total	**16**	**8**	**24**	**280**	**120**	**400**
VII	Major	CHEM401C16	Advanced Spectroscopy	4		4	35	15	50 (T)
VII	Major	CHEM402C17	Advanced Physical Chemistry	4		4	35	15	50 (T)
VII	Major	CHEM403C18	ORGANIC CHEMISTRY-VI	4		4	35	15	50 (T)
VII	Major	CHEM441C19	Project Dissertation	4		4	50		50 (S)
VII	MC	CHEM442MC05	Research Methodology	4		4	50		50 (S)
			Semester-VII Total	**20**		**20**	**205**	**45**	**250**
VIII	Major	CHEM451C20	Soft Materials, Nanomaterials and Advanced Functional Materials	4		4	35	15	50 (T)
VIII	Major	CHEM452C21	INORGANIC CHEMISTRY-VI	4		4	35	15	50 (T)
VIII	Major	CHEM453C22	ORGANIC CHEMISTRY-VII	4		4	35	15	50 (T)
VIII	Major	CHEM491C23	Project Dissertation	8		8	100		100 (S)
VIII	MC	CHEM492MC06	Research and Publication Ethics	4		4	50		50 (S)
			Semester-VIII Total	**24**		**24**	**255**	**45**	**300**
			Total			**194**			**3000**

* MC = Minor Course, MDC = Multi-Disciplinary Course, SEC = Skill Enhancement Course, AECC = Ability Enhancement Compulsory Course, VAC = Value Added Course, Th. = Theory, Pr. = Practical, CA = Continuous Assessment T = Taught Paper, S = Sessional Paper

Structure of Chemistry Courses

Semester		Number of Course					
	Major	AECC	SEC (out of)	VAC	MC	MDC	Summer Internship
1st	2	1	-	-	1	1	-
2nd	2	1	-	-	1	2	-
3rd	2	-	1 (2)	1	1	-	-
4th	2	-	1 (2)	1	1	-	-
5th	3	-	-	-	-	-	1
6th	4	-	-	-	-	-	-
7th	4	-	-	-	1	-	-
8th	4	-	-	-	1	-	-
Total	**23**	**2**	**2**	**2**	**6**	**3**	**1**

SEMESTER- I

CHEM101C01: INORGANIC CHEMISTRY-I

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Course Objectives: The course aims to provide the knowledge on atomic structure, periodic table, periodic properties of elements, various types of chemical bonding in molecule, elementary idea of redox chemistry. Basic idea on the laboratory instruments, and titration techniques in laboratory experiments.

Atomic Structure:

Bohr's theory, its limitations and atomic spectrum of hydrogen atom. Sommerfeld modification. Wave mechanics: de Broglie equation, Heisenberg's Uncertainty Principle and its significance, Schrödinger's wave equation. Hydrogenic wavefunctions, Quantum numbers, introduction to the concept of atomic orbitals; shapes, radial and angular probability diagrams of s, p and d orbitals (qualitative idea). Many electron atoms and ions: Pauli's exclusion principle, Hund's rule, exchange energy, Aufbau principle and its limitations. Term symbols of atoms and ions. **(14 Lectures)**

Periodicity of Elements:

s, *p*, *d*, *f* block elements, the long form of periodic table. Detailed discussion of the following properties of the elements, with reference to *s* and *p*-block – group trend and periodic trend.

(a) Effective nuclear charge, shielding or screening effect, Slater rules, variation of effective nuclear charge in periodic table.

(b) Atomic radii (van der Waals)

(c) Ionic and crystal radii.

(d) Covalent radii (octahedral and tetrahedral)

(e) Ionization enthalpy, Successive ionization enthalpies and factors affecting ionization energy. Applications of ionization enthalpy.

(f) Electron gain enthalpy, trends of electron gain enthalpy.

(g) Electronegativity, Pauling's/ Mulliken's/ Allred Rachow's/ and Mulliken-Jaffé's electronegativity scales. Variation of electronegativity with bond order, partial charge, hybridization, group electronegativity. **(16 Lectures)**

Chemical Bonding:

(i) *Ionic bond:* General characteristics, types of ions, size effects, radius ratio rule and its limitations. Packing of ions in crystals. Born-Landé equation with derivation and importance of Kapustinskii expression for lattice energy. Madelung constant, Born-Haber cycle and its application, Solvation energy.

(ii) *Covalent bond:* Lewis structure, Valence Bond theory (Heitler-London approach). Hybridization, equivalent and non-equivalent hybrid orbitals. Bent's rule, Resonance and resonance energy, Molecular orbital theory. Molecular orbital diagrams of diatomic and simple polyatomic molecules N_2, O_2, C_2, B_2, F_2, CO, NO, HCl,

BeF_2, CO_2, (idea of s-p mixing and orbital interaction to be given). Formal charge, Valence shell electron pair repulsion theory (VSEPR), shapes of simple molecules and ions containing lone pairs and bond pairs of electrons, multiple bonding (σ and π bond approach) and bond lengths.

Covalent character in ionic compounds, polarizing power and polarizability. Fajan's rule and consequences of polarization.

Ionic character in covalent compounds: Bond moment and dipole moment. Percentage ionic character from dipole moment and electronegativity difference.

(iii) *Metallic Bond:* Qualitative idea of valence bond and band theories. Semiconductors and insulators, defects in solids. **(20 Lectures)**

Oxidation-Reduction:

Elementary idea on standard redox potentials with sign convention, Nernst equation. Influence of complex formation, precipitation and change of pH on redox potentials, formal potential. Feasibility of a redox titration, redox potential at the equivalence point, redox indicators, redox potential diagram (Latimer and Frost) of common elements and their applications. Disproportionation and comproportionation reactions (typical examples). **(10 Lectures)**

Reference Books:

- Lee, J.D. Concise Inorganic Chemistry ELBS, 1991.
- Douglas, B.E. and McDaniel, D.H. Concepts & Models of Inorganic Chemistry Oxford, 1970
- Rodger, G.E. Inorganic and Solid State Chemistry, Cengage Learning India Edition, 2002.
- R. L. Dutta & G.S. De, Inorganic Chemistry (Vol. 1), The New Book Stall, 1973.
- Atkin, P. Shriver & Atkins' Inorganic Chemistry 5th Ed. Oxford University Press, 2010.
- R. P. Sarkar, General and Inorganic Chemistry (Vol. 1), New Central Book Agency, ed. 3, 2011
- A. K. Das, Fundamental Concepts of Inorganic Chemistry (Vol. 1,2 and 3), CBS Publishers & Distributors, 2010
- Huheey, J. E.; Keiter, E.A. & Keiter, R.L. Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed., Harper Collins 1993, Pearson,2006.

CHEMISTRY PRACTICAL- CHEM101C01 LAB:

(Credits: Practicals-02, 60 Lectures, Full marks: 30)

Elementary idea of redox titration using $KMnO_4$ and $K_2Cr_2O_7$

A. Acid-Base Titrations

1. Estimation of carbonate and hydroxide present together in mixture.
2. Estimation of carbonate and bicarbonate present together in a mixture.

B. Redox Titrations

B-1. **Redox Titrimetric Estimations Based on Permanganometry**

1. Estimation of Fe(III) and Fe(II) mixture.
2. Estimation of Fe (III) and Ca (II) in a mixture

B-2. **Redox Titrimetric Estimations with standard $K_2Cr_2O_7$ solution**

1. Estimation of Fe(III) and Fe(II) mixture.
2. Estimation of Fe (III) and Cu (II) in a mixture

Reference Book:

- Mendham, J., A. I. Vogel's Quantitative Chemical Analysis 6th Ed., Pearson, 2009.
- G. N. Mukherjee, Hand Book of Inorganic Analysis, U. N. Dhar & sons (P) LTD, 2014

Course Learning Outcomes:

On completion of the course, the students should be able to

1. Explain dual nature of subatomic particles. They will also gain preliminary notion about quantum mechanical model of the atom and shape of s, p, d, and f-orbitals.
2. Distinguish the types of bonding in a molecule and rationalize qualitative idea of valence bond and band theories.
3. Demonstrate the underlying concepts of periodic table developments and various periodic properties such as atomic size, ionization energy, electronegativity, electron affinity, etc… Changes of these periodic properties across the period and down the group.
4. Draw the molecular orbital energy diagram for some selected homo- & hetero nuclear diatomic molecules.
5. Predict structure and geometries of inorganic compounds; assign electrons to respective orbitals and shells to determine the electronic configuration of a particular element.

They will be able to determine the redox potential of a given redox couple to predict the feasibility of a reaction.

6. Learn about the safety protocols inside a chemistry lab. They will be able to prepare solutions with desired strength and can to analyse the concentration of unknown samples using titrations.

CHEM102C02: PHYSICAL CHEMISTRY-I

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Course Objectives: To impart knowledge on the kinetic theory of gas, behaviour of real gas, viscosity of gas and liquid, solid state chemistry and fundamentals of thermodynamics.

Gaseous state: Kinetic molecular model of a gas: postulates and derivation of the kinetic gas equation; The Barometric distribution law; Maxwell distribution and its use in evaluating molecular velocities (average, root mean square and most probable) and average kinetic energy, idea about gamma function and related integral, error function, Maxwell distribution for kinetic energy, Maxwell –Boltzmann distribution law; law of equipartition of energy, degrees of freedom and molecular basis of heat capacities.

Collision frequency; collision diameter; mean free path and viscosity of gases, including their temperature and pressure dependence, relation between mean free path and coefficient of viscosity, calculation of σ from η; variation of viscosity with temperature and pressure. Kinetic theory of gas in interpreting Fick's law of diffusion and Fourier law of heat conduction.

Behaviour of real gases: Deviations from ideal gas behaviour, Andrew's and Amagat's plots); compressibility factor, *Z*, and its variation with pressure for different gases. Causes of deviation from ideal behaviour. Van der Waals equation of state, its derivation and application in explaining real gas behaviour, mention of other equations of state (Berthelot, Dieterici); virial equation of state; van der Waals equation expressed in virial form and calculation of Boyle temperature. Isotherms of real gases and their comparison with van der Waals isotherms, continuity of states, critical state, relation between critical constants and van der Waals constants, law of corresponding states;

Intermolecular forces and potentials (Keesom, Debye and London), estimation of van der Waals constants, Lennard-Jones potential.

(20 Lectures)

Viscosity of liquid: Qualitative treatment of the structure of the liquid state; physical properties of liquids; vapour pressure. General features of fluid flow (streamline and turbulent flows, Reynold's number); nature of viscous drag for streamline motion, Newton's equation, viscosity coefficient, Poisuille equation (with derivation), coefficient of viscosity. Stokes' law and terminal velocity; experimental determination of viscosity coefficient of liquids. Stokes'-Einstein relation for diffusivity, Effect of addition of various solutes viscosity. Temperature variation of viscosity of liquids and comparison with that of gases. Qualitative discussion of

structure of water (qualitative idea).

(8 Lectures)

Chemical Thermodynamics:

Importance and scope, intensive and extensive variables; state and path functions; isolated, closed and open systems; zeroth law of thermodynamics.

First law: Concept of heat, *q*, work, *w*, internal energy, *U*, and statement of first law; enthalpy, *H*, heat changes at constant volume and constant pressure; relation between C_p and C_v using ideal gas and van der Waals equations; joule's experiment and its consequence; explanation of term $(\delta U/\delta V)_T$, calculations of *q*, *w*, ΔU and ΔH for reversible, irreversible and free expansion of gases (ideal and van der Waals) under isothermal and adiabatic conditions.

Thermochemistry: Heats of reactions: standard states; enthalpy of formation of molecules and ions and enthalpy of combustion and its applications; calculation of bond energy, bond dissociation energy and resonance energy from thermochemical data, effect of temperature (Kirchhoff's equations) and pressure on enthalpy of reactions. Adiabatic flame temperature, explosion temperature.

Second Law: Second law of thermodynamics: need for a second law, Clausius and Kelvin-Planck statements and their equivalence; Carnot's theorem, thermodynamic scale of temperature, concept of heat engine, Carnot cycle and refrigerator; Concept of entropy; Clausius inequality, entropy as a state function, second law in terms of entropy, molecular and statistical interpretation of entropy. Calculation of entropy change for reversible and irreversible processes.

Free Energy Functions: Gibbs and Helmholtz energy; variation of S, G, A with T, V, P; Free energy change and spontaneity. Relation between Joule-Thomson coefficient and other thermodynamic parameters; inversion temperature; Gibbs-Helmholtz equation; Maxwell relations; thermodynamic equation of state.

(24 Lectures)

Systems of Variable Composition:

Partial molar quantities, dependence of thermodynamic parameters on composition; Gibbs-Duhem equation, Eulers theorem. Non-ideal system: Excess thermodynamic functions, idea of fugacity and activity; standard states. chemical potential of ideal mixtures, change in thermodynamic functions in mixing of ideal gases. Activity coefficient for electrolytes, Debye Huckel theory (preliminary idea).

(8 Lectures)

Reference Books:

- Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry 10th Ed., Oxford University Press (2014).
- Ball, D. W. Physical Chemistry Thomson Press, India (2007).
- Castellan, G. W. Physical Chemistry 4th Ed. Narosa (2004).
- Mortimer, R. G. Physical Chemistry 3rd Ed. Elsevier: NOIDA, UP (2009).
- Engel, T. & Reid, P. Physical Chemistry 3rd Ed. Pearson (2013).

CHEMISTRY PRACTICAL-CHEM102C02 LAB

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

1. Viscosity measurement using Ostwald's viscometer.

(a) Determination of viscosity of aqueous solutions of (i) polymer (ii) ethanol and (iii) sugar at room temperature.

(b) Study the variation of viscosity of sucrose solution with the concentration of solute.

2. Thermochemistry

(a) Determination of heat capacity of a calorimeter for different volumes using change of enthalpy data of a known system (method of back calculation of heat capacity of calorimeter from known enthalpy of solution or enthalpy of neutralization).

(b) Determination of heat capacity of the calorimeter and enthalpy of neutralization of hydrochloric acid with sodium hydroxide.

(c) Calculation of the enthalpy of ionization of ethanoic acid.

(d) Determination of heat capacity of the calorimeter and integral enthalpy (endothermic and exothermic) solution of salts.

(e) Determination of enthalpy of hydration of copper sulphate.

(f) Study of the solubility of benzoic acid in water and determination of ΔH.

Reference Books

- Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011).
- Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry 8th Ed.; McGraw-Hill: New York (2003).
- Halpern, A. M. & McBane, G. C. Experimental Physical Chemistry 3rd Ed.; W.H. Freeman & Co.: New York (2003).

Course Learning Outcomes: After the completion of the course, the students should be able to

1. Explain the kinetic molecular model of gas, viscosity of gas and liquids.
2. Manipulate the gas laws to describe real and ideal gas behaviour.
3. Describe the Three Laws of Thermodynamics and their development.

4. Perform the experiments to measure the heat of reaction
5. Demonstrate the basic idea about the direction of physical and chemical processes in terms of thermodynamic parameters
6. Use the Maxwell equations and other thermodynamic relations to compute thermodynamic quantities from thermodynamic data tables.
7. Apply the concept of chemical potential to explain the Gibbs free energy change due to mixing and calculate partial molar quantities.

CHEM104MC01

Theory: Atomic Structure, Bonding, General Organic Chemistry, Aliphatic Hydrocarbons

(Credits: 04, 60 Lectures, Full Marks: 70)

Course Objectives: The course aims to provide the knowledge on atomic structure, and various types of chemical bonding in molecule to general science students, basic idea on titration techniques in laboratory experiments.

Section A: Inorganic Chemistry

Atomic Structure:

Extra-nuclear Structure of atoms Bohr's theory for hydrogen atom (simple mathematical treatment), atomic spectra of hydrogen, quantum numbers and their significance, Pauli's exclusion principle, Hund's rule, electronic configuration of many- electron atoms, Aufbau principle and its limitations.

Stability of half-filled and completely filled orbitals, concept of exchange energy. Relative energies of atomic orbitals, Anomalous electronic configurations. **(14 Lectures)**

Chemical Bonding and Molecular Structure:

*Ionic bonding:*General characteristics of ionic compounds, sizes of ions, radius ratio rule and its limitation. Lattice energy, Born Haber cycle.

Covalent bonding: General characteristics of covalent compounds, valence-bond approach, hybridization involving s, p, d orbitals. Valence Shell Electron Pair Repulsion (VSEPR) concept, shapes of simple molecules and ions of main group elements, bond moment and dipole moment, partial ionic character of covalent bonds, Fajan's rules, hydrogen bonding and its effect on physical and chemical properties.

MO Approach: Rules for the LCAO method, bonding and antibonding MOs and their characteristics for s-s, s-p and p-p combinations of atomic orbitals, nonbonding combination of orbitals, MO treatment of homonuclear diatomic molecules of 1st and 2nd periods (including idea of s-p mixing) and heteronuclear diatomic molecules such as CO and NO. **(16 Lectures)**

Section B: Organic Chemistry

Course Objectives: To impart knowledge on fundamentals of organic chemistry, stereochemistry of organic compounds and aliphatic hydrocarbons

Fundamentals of Organic Chemistry

Physical Effects, Electronic Displacements: Inductive Effect, Electromeric Effect, Resonance and Hyperconjugation. Cleavage of Bonds: Homolysis and Heterolysis. Structure, shape and reactivity of organic molecules: Nucleophiles and electrophiles. Reactive Intermediates: Carbocations, Carbanions and free radicals. Strength of organic acids and bases: Comparative study with emphasis on factors affecting pK values. Aromaticity: Benzenoids and Hückel's rule. **(8 Lectures)**

Stereochemistry

Conformations with respect to ethane, butane, and cyclohexane. Interconversion of Wedge Formula, Newman, Sawhorse and Fischer representations. Concept of chirality (upto 2 carbon atoms). Geometrical and optical isomerism, Enantiomerism, diastereomerism and *meso*-compounds. *Threo/erythron, D/L, cis-/trans, R/S, E/Z*-nomenclature, and CIP rules.

(10 Lectures)

Aliphatic Hydrocarbons

Alkanes: Preparation – Catalytic hydrogenation (*cis-/trans*-addition of hydrogen, Birch reduction, heats of hydrogenation), Wurtz reaction, Kolbe's synthesis, from Grignard reagent (with mechanism). Reactions – Free radical substitution (Halogenation).

Alkenes: Preparation *via* elimination reactions – Dehydration of alcohols, Dehydrohalogenation of alkyl halides, Elementary idea to *E1, E2*-eliminations, Stereochemical requirement for *E2*, Saytzeff and Hofmann rule, Effect of bulky bases, *cis*- and *trans*-alkenes. Reactions – *Syn*-dihydroxylation by OsO_4, alkaline $KMnO_4$, bromination (*anti*-addition), hydration, ozonolysis, Markownikoff's and anti-Markownikoff's rule, addition of HX, Oxymercuration-demercuration, Hydroboration-oxidation.

Alkynes: Preparation – Acetylene from CaC_2 and conversion into higher alkynes, by dehalogenation of tetrahalides, and dehydrohalogenation of *vic*-dihalides. Reactions – hybridization effect on the acidity of hydrocarbons, formation of metal acetylides, alkylation of terminal alkynes, halogenation, ozonolysis, and oxidation with hot alkaline $KMnO_4$.

(12 Lectures)

Reference Books:

- Lee, J. D. Concise Inorganic Chemistry, ELBS (1991).
- Dutta, R. L. & De, G. S. Inorganic Chemistry (Vol. 1), The New Book Stall (1973).
- Sarkar, R. P. General and Inorganic Chemistry (Vol. 1), 3rd Ed., New Central Book Agency (2011).
- Sykes, P. A Guidebook to Mechanism in Organic Chemistry, Orient Longman, New Delhi, (1988).
- Eliel, E. L. Stereochemistry of Carbon Compounds, Tata McGraw Hill Education (2000).
- Graham Solomons, T. W.; Fryhle, C. B. & Snyder, S. A. Organic Chemistry, 12th Ed., John Wiley & Sons (2017).
- Finar, I. L. Organic Chemistry (Vol. I), 6th Ed., Pearson (2002).

CHEM104MC01-Lab:

(Credits: 02, 60 Lectures, Full Marks: 30)

Section A: Inorganic Chemistry - Volumetric Analysis (any four)

1. Estimation of sodium carbonate and sodium hydrogen carbonate present in a mixture.
2. Estimation of oxalic acid by titration with $KMnO_4$.
3. Estimation of water of crystallization in Mohr's salt by titration with $KMnO_4$.
4. Estimation of Fe(II) ions by titration with $K_2Cr_2O_7$.
5. Estimation of Cu(II) ions iodometrically using $Na_2S_2O_3$.

Section B: Organic Chemistry

1. Detection of extra elements (N, S, Cl, Br, I) in organic compounds.

2. Separation of mixtures by Chromatography: Measurement of R_f value in each case (combination of two compounds to be given)

(a) Separate and identify the aromatic compounds in a given mixture by Thin Layer Chromatography

(b) Separate and identify the components of a given mixture of two amino acids (glycine, aspartic acid, glutamic acid, tyrosine, or any other amino acid) by paper chromatography.

(c) Separate and identify the sugars present in a given mixture by paper chromatography.

Reference Books:

- Svehla, G. *Vogel's Qualitative Inorganic Analysis*, Pearson Education, 2012.
- Mendham, J. *Vogel's Quantitative Chemical Analysis*, Pearson, 2009.
- Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J. & Smith, P.W.G., *Textbook of Practical Organic Chemistry*, Prentice-Hall, 5th edition, 1996.
- Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry* Orient-Longman, 1960.

Course Learning Outcomes: On completion of the course, the students should be able to

1. Explain the dual nature of subatomic particles. They will also gain a preliminary notion about the quantum mechanical model of the atom and the shape of s, p, d, and f-orbitals.
2. Distinguish the types of bonding in a molecule and rationalize the qualitative idea of valence bond and band theories.
3. Prepare solutions with the desired strength and analyse the concentration of unknown samples using titrations.

4. Interpret the physical and chemical properties of organic molecules to predict their reactivity, nature of reactive intermediates, and various reaction mechanisms.
5. Explain the geometrical and optical isomerism; execute interconversion of different 3D- and 2D-projections of saturated organic molecules along with their stereochemical nomenclature.
6. Elucidate several preparative routes and reactions of aliphatic hydrocarbons.
7. Identify special elements present in organic samples and perform chromatographic separations to detect constituents of a supplied mixture.

CHEM105MDC01: Chemistry in everyday life

(Credits: 03, Theory-03, 30 Lectures, Full Marks: 50)

Course Objectives: The course aims to provide the knowledge on Chemistry in daily life

Chemistry in agriculture:

Fertilizers- nitrogenous, phosphatic and potassium fertilizers, organic fertilizers, deficiency symptoms of micro and macronutrients

Pesticides: Introduction, types of pesticides, importance of pesticides, natural and artificial pesticides, toxic effects of pesticides.

Chemistry of Food additives and preservatives: antioxidants and radical scavengers, emulsifiers stabilisers, gums, thickeners and gelling agents as food additives, sweeteners, fragrances, flavouring agents and enhancers, food acids and acidity regulators, food colour and colour retention agents, flour treatment/improving agents, anticaking agents, minerals and mineral salts, dietary supplements

Chemistry of food Preservatives: Reasons for food deterioration, why preservatives necessary, permissible limit, classes of preservatives, brief overview of some commonly used preservatives, mode of action of chemical preservatives, -pasteurisation of packaged foods, pasteurisation of unpackaged liquid foods, -quality assurance

Food adulteration: Introduction, foods commonly adulterated, common adulterants, classification of adulterants, harmful effects of some adulterants

Chemistry of cosmetics and personal care products: definition of cosmetics, history of cosmetics and natural products, broad classification of cosmetics, brief overview of emulsions, surfactants, emollients, moisturizers, waxes, thickeners, active ingredients, sunscreens, color, preservatives

Chemical composition and formulation of skin creams and lotions, shaving cream, sunscreen, lips-stick and lip balms, eye-makeup. Cosmetic formulation, chemistry of hair care, skin care, color cosmetics, and sun protections. Chemistry of perfumes and fragrances, deodorants and antiperspirants. Chemistry of toothpaste, composition of toothpaste.

Chemistry of commonly used Drugs: Drugs and their Classification, Drug-Target Interaction, Therapeutic Action of Different Classes of Drugs such as: Antacids, Antihistamines, Neurologically Active Drugs (Tranquilizer, analgesic), Antimicrobials (Antibiotic, Antiseptic, Disinfectant), Antifertility Drugs

Chemistry of Soap and Detergents: Introduction to soaps and detergents, properties, comparison between soap and detergents, types of soap, behaviour in hard water, synthetic detergents, classification, preparation overview of soap and detergents.

(30 Lectures)

References

- Sharma, B. K. Industrial Chemistry (volume 1&2), Krishna Prakashan Media, Meerut (2016).

- Jain, P. C., Jain, M. Engineering Chemistry, Dhanpat Rai & Sons, Delhi (2015).
- Saha, C., Chakraborty, B., Basu, K., Chakraborty, S. Lectures on Pharmaceutical Chemistry and Pesticide Chemistry, Techno World (2020).
- Chopra, H. K., Panesar, P. S. Food Chemistry, Narosa Publishing House, New Delhi (2010)

Course Learning Outcomes: After completion of the course, the student should be able to

1. Visualise the importance of Chemistry in daily life
2. Explore the application of different chemicals in daily life.

SEMESTER- II

CHEM151C03: INORGANIC CHEMISTRY-II

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Course Objectives: The course aims to provide the knowledge on introduction to coordination compounds, general chemistry of the elements and their periodic properties, and also some **industrial applications** of different compounds of some important elements e.g. Silicones, phosphazenes. **Environmental** hazards like CFCs are also included to create awareness. comparison of inherent properties of transition metals in group, lanthanides and actinides

Basic Concepts of Coordination Chemistry:

Werner's theory, IUPAC nomenclature of coordination compounds, isomerism in coordination compounds. Stereochemistry of complexes with 4 and 6 coordination numbers. valence bond theory (inner and outer orbital complexes), electroneutrality principle and back bonding. Crystal field theory, measurement of 10 Dq (Δo), CFSE in weak and strong fields, pairing energies, factors affecting the magnitude of 10 Dq (Δo, Δt). Octahedral vs. tetrahedral coordination, tetragonal distortions from octahedral geometry Jahn-Teller theorem, square planar geometry **(14 Lectures)**

Chemistry of *s* and *p* Block Elements:

Inert pair effect, relativistic effect, relative stability of different oxidation states, diagonal relationship and anomalous behaviour of first member of each group. Allotropy and catenation. Complex formation tendency of *s* and *p* block elements. Basic properties of halogens. Hydrides and their classification ionic, covalent and interstitial. (**4 lectu**res)

Industrially important Inorganic Chemicals

Study of the following compounds with emphasis on structure, bonding, preparation, properties and uses: crown ethers and cryptates of Group I; basic beryllium acetate, beryllium nitrate, EDTA complexes of calcium and magnesium. Solutions of alkali metals in liquid ammonia and their properties, Boric acid and borates, borohydrides (diborane), carboranes, graphitic compounds, silanes, oxides and oxoacids of nitrogen, phosphorus and chlorine, halides of silicon and phosphorous, peroxo acids of sulphur, interhalogen compounds, polyhalide ions, pseudohalogens. **(14 lectures)**

Noble Gases:

Occurrence, large scale production and uses of noble gases, rationalization of inertness of noble gases, Clathrate compounds of noble gases, structure and bonding of oxo-, fluoro and fluoro-oxo compounds of xenon, xenate ions **(4 lectures)**

Inorganic Polymers:

Types of inorganic polymers, general properties of inorganic polymers, comparison with organic polymers. Synthesis, structural aspects and applications of the following polymer: Borazine, substituted borazines, phosphazenes, polyphosphates, polyphosphoesters, silicones, siloxanes, silicates, Polymeric compounds of sulphur and nitrogen.

Pre-ceramic Inorganic polymers: Silicon carbide, Boron nitride, Aluminium nitride, Phosphorous nitride. **(8 lectures)**

Chemistry of d- and f-Block Elements

d-block elements: General comparison of 3d, 4d and 5d elements; Elemental form; Electronic configuration; Oxidation state; Redox properties; Atomic radii; Ionization potentials; Metallic nature; Atomization energy; Coordination chemistry and catalytic properties

f-block elements: Lanthanides: Lanthanide contraction; Electronic configuration; Oxidation states; Atomic/Ionic radii; Ionization energy; Complex formation; Isomerization; Basicity; Hydration of Ln (III) ions; Organometallics compounds and their applications; Separation of lanthanides by ion exchange method; **Actinides:** Actinide contraction; Electronic configuration; Oxidation states; Atomic/Ionic radii; Ionization energy; Complex formation and Organometallics compounds, Super heavy elements; Applications of lanthanides and actinides

(16 Lectures)

Reference Books:

- W. U. Malik, G. D. Tuli, R. D. Madan, Selected Topics in Inorganic Chemistry, S. Chand Publishers, 2001
- R. L. Dutta & G.S. De, Inorganic Chemistry (Vol. 1), The New Book Stall, 1973.
- Purcell, K.F & Kotz, J.C. Inorganic Chemistry W.B. Saunders Co, 1977.
- Huheey, J. E.; Keiter, E.A. & Keiter, R.L. Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed., Harper Collins 1993, Pearson, 2006.
- Lee, J.D. Concise Inorganic Chemistry, ELBS, 1991.
- Douglas, B.E; Mc Daniel, D.H. & Alexander, J.J. Concepts & Models of Inorganic Chemistry 3rd Ed., John Wiley Sons, N.Y. 1994.
- Cotton, F.A. & Wilkinson, G, Advanced Inorganic Chemistry Wiley-VCH, 1999
- Greenwood, N.N. & Earnshaw. Chemistry of the Elements, Butterworth-Heinemann. 1997.
- Miessler, G. L. & Donald, A. Tarr. Inorganic Chemistry 4th Ed., Pearson, 2010.
- Atkin, P. Shriver & Atkins' Inorganic Chemistry 5th Ed. Oxford University Press (2010).
- R. P. Sarkar, General and Inorganic Chemistry (Vol. 1), New Central Book Agency, ed. 3, 2011
- Asim K. Das Fundamental Concepts of Inorganic Chemistry, Vol-1, 2 and 3
- Huheey, J. E.; Keiter, E.A. & Keiter, R.L. Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed., Harper Collins 1993, Pearson,2006.
- The f Elements by Nikolas Kaltsoyannis and Peter Scott

CHEMISTRY PRACTICAL – CHEM151C03 LAB

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

A. Inorganic preparations (Minimum Three)

1. Cuprous Chloride
2. Preparation of Manganese (III) phosphate
3. Preparation of Aluminium potassium sulphate (Potash alum) or Chrome alum.
4. Tetraamminecopper(II) sulphate
5. *Cis*- and *trans*- Potassium dioxalatodiaquachromate(III)
6. Tetraamminecarbonatocobalt(III) ion
7. Potassium tris(oxalate)ferrate(III)

B. Paper Chromatography (Any two)

1. Ni(II) and Co(II)
2. Fe(III) and Al(III)
3. Ni(II), Mn(II), Co(II) and Zn(II)

C. Gravimetric Analysis (Any One):

1. Estimation of nickel (II) using dimethylglyoxime.
2. Estimation of copper as CuSCN
3. Estimation of Al(III) by precipitating with oxine and weighing as $Al(oxine)_3$ (aluminiumoxinate).

Reference Book:

- Mendham, J., A. I. Vogel's Quantitative Chemical Analysis 6th Ed., Pearson, 2009.
- S. Gulati, J. L. Sharma, S. Manocha, Practical Inorganic Chemistry, CBS Publishers distributers, 2017.

Course Learning Outcomes: After the completion of the course, the students should be able to

1. Differentiate double-salts and coordination complexes.
2. Explain the structure, spectral and magnetic properties of coordination complexes
3. Predict spectral properties using various theory of coordination chemistry
4. Demonstrate the periodic properties of d and f block elements
5. Use the Periodic Table to rationalize similarities and differences of elements, including physical and chemical properties and reactivity.
6. Have good knowledge of some industrial applications of some elements.

7. Have good knowledge of Periodicity of the group elements
8. Have good knowledge of special properties like relativistic effects of rare elements.
9. They may also have handful of experience on handling the various apparatus involved on synthesis of inorganic compounds as well as some redox titration

CHEM152C04: ORGANIC CHEMISTRY- I

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Course Objectives: To impart knowledge on fundamentals of organic chemistry, structure, reactivity, kinetics, and stereochemistry of organic compounds and investigation of reaction mechanism.

Basics of Organic Chemistry, Chemical bonding & Reaction Mechanism

Organic Compounds: Classification, Hybridization, Shapes of molecules, Influence of hybridization on bond properties (VBT).

Electronic Effects: Inductive, Electromeric, Resonance and Mesomeric effects, Hyperconjugation and their applications. Dipole moment, Organic acids, bases and their relative strengths.

Reaction Mechanism: Homolytic and Heterolytic fission with suitable examples, Reaction Mechanism (ionic and radical), Representation of mechanistic steps using arrow formalism, and formal charges. Reactive intermediates – carbocations (carbenium and carbonium ions), carbanions, carbon radicals, carbenes, and nitrenes – structure using orbital picture.

Reaction kinetics: Rate constant and Free energy of activation, Free energy profiles for one step and multistep reactions, Catalyzed reactions, Kinetic and thermodynamic control, Kinetic isotopic effect, Principle of microscopic reversibility, Hammond postulate.

(20 Lectures)

Stereochemistry

***Molecular Symmetry and Chirality*:** Symmetry operations, Symmetry elements and Point group classification.

Stereoisomerism: Definition, Classification, Molecular representation using Fischer, Newman, Sawhorse and Flying wedge projection formulae and their interconversions. Enantiomers, Diastereomers, *meso*-structures, Racemic modifications, and methods of resolution. Optical activity, Specific rotation, Centre of chirality, Relative and Absolute configuration, Configurational nomenclature: *D/L, R/S, E/Z, erythro/threo, pref/parf, like/unlike, cis/trans,* and *syn/anti*, C.I.P rules, Constitutionally unsymmetrical and symmetrical chiral molecules.

Axial Chirality: Stereochemistry of allenes, spiranes and analogues, Biphenyl derivatives and atropisomerism, bridged biphenyls and configurational nomenclature.

Topocity: Homotopic, enantiotopic and diastereotopic ligands and faces, and their recognition.

Conformations of monocyclic compounds: Conformational analysis of cyclopropane, cyclobutane, cyclopentane, and cyclohexane: Geometry, relative stability, energy diagrams of cyclohexane and substituted cyclohexanes: Chair, Boat and Twist boat forms.

(20 Lectures)

Substitution and Elimination Reactions

Nucleophilic substitution reactions at sp^3 centre: S_N1, S_N2, S_N2', S_N1' and S_Ni mechanisms, Effect of substrate structure, Leaving group, Solvent and Nucleophiles including ambident nucleophiles, Nucleophilicity and basicity, substitution involving NGP (with hetero atoms and aryl groups), Relative rate & stereochemical features – role of crown ethers and phase transfer catalysts (systems: alkyl halides, allyl halides, benzyl halides, alcohols, ethers, epoxides, α-halocarbonyls). Relative reactivity of alkyl, allyl/benzyl, vinyl halides towards nucleophilic substitution reactions.

Elimination reactions: Formation of alkenes and alkynes by elimination reactions, Mechanism of E1, E2, E1cB, E_i (pyrolytic *syn*-elimination) reactions, Regioselectivity (Saytzeff and Hofmann eliminations) and stereoselectivity. Substitution *vs*. elimination.

(20 Lectures)

Reference Books:

- Smith, M. B. *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, 8th Ed., Wiley (2020).
- Graham Solomons, T. W.; Fryhle, C. B. & Snyder, S. A. *Organic Chemistry*, 12th Ed., John Wiley & Sons (2017).
- Finar, I. L. *Organic Chemistry (Vol. I)*, 6th Ed., Pearson (2002).
- Nasipuri, D. *Stereochemistry of Organic Compounds*, New Age International (P) Ltd. (1991).
- Eliel, E. L. & Wilen, S. H. *Stereochemistry of Organic Compounds*, Wiley: London (1994).
- Sykes, P. *A Guidebook to Mechanism in Organic Chemistry*, Pearson (2003).

CHEMISTRY PRACTICAL – CHEM152C04 LAB

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

1. Purification of organic compounds by crystallization using (a) water, (b) alcohol and (c) alcohol-water.

2. Determination of the melting points of above compounds and unknown organic compounds (using Kjeldahl method and melting point apparatus).

3. Effect of impurities on the melting point – mixed melting point of two unknown organic compounds.

4. Qualitative analysis of nitrogenous and non-nitrogenous functional groups for solid organic compounds.

5. Preparation of derivatives of the functional groups.

Reference Books:

- Mann, F. G. & Saunders, B. C. *Practical Organic Chemistry,* Pearson Education (2009).
- Furniss, B. S.; Hannaford, A. J.; Smith, P. W. G.; Tatchell, A. R. *Vogel's Textbook of Practical Organic Chemistry,* 5th Ed., Pearson Education (2012).

Course Learning Outcomes: After completion of the course, the student should be able to

1. Analyse different physical and chemical properties of organic molecules related to their reactivity, nature of reactive intermediates, and various kinds of reaction mechanisms: Elimination and Substitution.
2. Quantify reaction parameters through real instances.
3. Interpret geometrical and stereoisomerism, their role in physical and chemical properties of organic molecules, describe 3D-structures of saturated organic molecules and their projections on 2D-plane and concepts of central and axial chirality; explain conformational analysis of cyclic and acyclic systems.
4. Purify organic solids, and detect various functional groups present in organic samples which will improve their analytical skills.

CHEM154MC02

Theory: Chemical Energetics, Equilibria & Functional Organic Chemistry

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Section A: Physical Chemistry

Course Objectives: To impart knowledge on the basic concepts of classical thermodynamics and its application on chemical and ionic equilibrium.

Chemical Energetics

Review of thermodynamics and the Laws of Thermodynamics. Important principles and definitions of thermochemistry. Concept of standard state and standard enthalpies of formations, Integral and differential enthalpies of solution and dilution. Calculation of bond energy, Bond dissociation energy and Resonance energy from thermochemical data. Variation of enthalpy of a reaction with temperature – Kirchhoff's equation. Statement of Third Law of thermodynamics and calculation of absolute entropies of substances.

(10 Lectures)

Chemical Equilibrium

Free energy change in a chemical reaction. Thermodynamic derivation of the law of chemical equilibrium. Distinction between ΔG and ΔG^{o}, Le Chatelier's principle. Relationships between Kp, Kc and Kx for reactions involving ideal gases.

(8 Lectures)

Ionic Equilibria

Strong, moderate and weak electrolytes, Degree of ionization, Factors affecting degree of ionization, Ionization constant and Ionic product of water. Ionization of weak acids and bases, pH scale, Common ion effect. Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions, Solubility and Solubility product of sparingly soluble salts – applications of solubility product principle.

(12 Lectures)

Section B: Organic Chemistry

Course Objectives: To impart knowledge on chemistry of aromatic hydrocarbons, alkyl and aryl halides, alcohols, phenols, ethers, and carbonyl compounds.

Aromatic hydrocarbons

Preparation of benzene – from phenol, by decarboxylation, from acetylene, from benzene sulphonic acid. Reactions of benzene – Electrophilic aromatic substitution (nitration, halogenation, sulphonation, Friedel-Craft's alkylation and acylation, and side chain oxidation of alkyl benzenes. **(8 Lectures)**

Alkyl and Aryl Halides

Alkyl Halides: Types of Nucleophilic Substitution (S_N1, S_N2 and S_Ni) reactions. Preparation from alkenes and alcohols. Reactions – hydrolysis, nitrite & nitro formation, nitrile & isonitrile formation. Williamson's ether synthesis, Elimination *vs* substitution.

Aryl Halides Preparation (Chloro, bromo and iodo-benzene): from phenol, Sandmeyer & Gattermann reactions. Reactions (Chlorobenzene): Aromatic nucleophilic substitution (replacement by –OH group) and effect of nitro substituent. Benzyne Mechanism: KNH_2/ liq. NH_3 (or $NaNH_2$/liq.NH_3). Reactivity and relative strength of C-Halogen bond in alkyl, allyl, benzyl, vinyl and aryl halides. **(8 Lectures)**

Alcohols, Phenols, Ethers, Aldehydes and Ketones

Alcohols: Preparation of 1°, 2° and 3° alcohols – using Grignard and organolithium reagents, Reduction of aldehydes, ketones, carboxylic acids and esters, Ester hydrolysis. Reactions – with sodium, Lucas test, esterification, oxidation (H_2CrO_4, alkaline $KMnO_4$, PCC/PDC), Oppenauer oxidation, Diols – oxidation of diols with HIO_4 and $Pb(OAc)_4$, Pinacol-Pinacolone rearrangement.

Phenols: Preparation – Hock process, from diazonium salts. Acidity of phenols. Reactions – Electrophilic aromatic substitutions: nitration, halogenation, sulphonation, Reimer-Tiemann formylation, Houben-Höesch acylation, Gattermann-Koch formylation, Schötten-Baümann Reaction.

Ethers (aliphatic and aromatic): Acidic cleavage of ethers.

Aldehydes and ketones (aliphatic and aromatic):

Preparation – from acid chlorides, esters, and nitriles. Reactions – Reaction with HCN, ROH, $NaHSO_3$, NH_2-G derivatives, haloform reaction, aldol condensation, Cannizzaro reaction, Wittig reaction, Benzoin condensation, Meerwein-Ponndorf-Verley reduction, Clemmensen reduction and Wolff-Kishner reduction. **(14 Lectures)**

Reference Books:

- Barrow, G. M. *Physical Chemistry,* Tata McGraw-Hill (2007).
- Castellan, G. W. *Physical Chemistry* 4th Ed., Narosa (2004).
- Kotz, J. C.; Treichel, P. M. & Townsend, J. R. *General Chemistry* Cengage Learning India Pvt. Ltd., New Delhi (2009).
- Mahan, B. H. *University Chemistry* 3rd Ed., Narosa (1998).
- Petrucci, R. H. *General Chemistry* 5th Ed., Macmillan Publishing Co.: New York (1985).
- Sykes, P. *A Guidebook to Mechanism in Organic Chemistry,* Orient Longman, New Delhi (1988).
- Finar, I. L. *Organic Chemistry (Vol. I)*, 6th Ed., Pearson (2002).
- Graham Solomons, T. W.; Fryhle, C. B. & Snyder, S. A. *Organic Chemistry,* 12th Ed., John Wiley & Sons (2017).
- Clayden, J.; Greeves, N.; Warren, S. & Wothers, P. *Organic Chemistry*, 2nd Ed., Oxford University Press (2012).
- Norman, R. O. C. & Coxon, J. M. *Principle of Organic Synthesis*, 2nd Ed., Springer (1993).

CHEM154MC02 Lab: (Credits: Practicals-02, 60 Lectures, Full Marks: 30)

Section A: Physical Chemistry

Thermochemistry

1. Determination of enthalpy of neutralization of HCl with NaOH.

2. Determination of enthalpy of ionization of acetic acid.

3. Study of the solubility of benzoic acid in water and determination of ΔH.

Ionic equilibria

pH measurements Measurement of pH of different solutions like aerated drinks, fruit juices, shampoos, and soaps (use dilute solutions of soaps and shampoos to prevent damage to the glass electrode) using pH-meter.

Preparation of buffer solutions:

(i) Sodium acetate-acetic acid

(ii) Ammonium chloride-ammonium hydroxide

Measurement of the pH of buffer solutions and comparison of the values with theoretical values.

Section B: Organic Chemistry

1. Purification of organic compounds by crystallization (from water and alcohol) and distillation.

2. Criteria of purity: Determination of melting and boiling points.

3. Preparations: Mechanism of various reactions involved to be discussed. Recrystallisation, determination of melting point and calculation of quantitative yields.

(a) Bromination of phenol/aniline.

(b) Benzoylation of amines/phenols.

(c) Oxime and 2,4-dinitrophenylhydrazone of aldehyde/ketone.

Reference Books:

- Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
- Mann, F. G. & Saunders, B. C. *Practical Organic Chemistry* Orient-Longman (1960).
- Vogel, A. I.; Tatchell, A. R.; Furnis, B. S.; Hannaford, A. J. & Smith, P. W. G. *Textbook of Practical Organic Chemistry*, 5th Ed., Prentice-Hall (1996).

Course Learning Outcomes: After completion of the course, the student should be able to

1. Describe the three Laws of Thermodynamics and their development.
2. Perform the experiments to measure the heat of reaction.
3. Demonstrate the basic idea regarding the direction of physical and chemical processes in terms of the thermodynamic parameters.
4. Measure the pH of different solutions like aerated drinks, fruit juices, shampoos, and soaps.
5. Explain the concepts of buffer solution and prepare buffer solution.
6. Describe differential behaviour of electron-rich and electron-deficient benzene rings toward electrophiles and nucleophiles.
7. Discuss on the preparative routes and reactions of alkyl and aryl halides.
8. Perform comparative studies between substitution and elimination pathways in substituted alkanes.
9. Acquaint with different functionalities like alcohols, phenols, ethers, and carbonyls in aliphatic and aromatic systems, and their reactions.
10. Preparation of simple organic molecules in one step and their purification.

CHEM155MDC02: Chemistry of Dyes, Colours, Application of Dyes and The Chemistry of Fireworks

(Credits: 03, Theory:03, 30 Lectures, Full Marks: 50)

Course Objectives: The course aims to provide the knowledge on History and Chemistry of Dyes, Colours and application of Dyes and paints.

To give a basic knowledge about the types of chemicals involved in the fireworks industry. To understand the importance of color producing chemicals in the fireworks industry and Safety measures.

Introduction to Dyestuff Chemistry: Important landmark in the history of dyes; Natural colouring matter and their limitations: e.g,; Heena, Turmeric, kesar, Chlorolphyll, Indigo, Alizarine.

Definition of dyes: Classification, **Principles of colour chemistry**, Chromophore and Auxochrome, Solubility, dyes versus pigments.

Colour and chemical constitution of dyes: Absorption of visible light, colour of wavelength absorbed, complementary colour; Relation between colour and chemical constitution:

Chemistry and synthesis of methylorange, Congo red, Malachite green, Crystal violet, Phenolphthalein and fluorescein, **Dyes and Indicators:** Phenolphthalein and fluorescein, Chemistry of dyeing: Mordant and Vat Dyes; Applications of dyes.

Natural dyes:Structure of Alizarin and Indigotin; **Edible Dyes** with examples.

Chemistry of paints: introduction and uses, properties of paint, brief overview of paints composition

The Chemistry of Fireworks:

Basics of Pyrotechnics/Fireworks, Electron transfer-Redox reaction, Thermochemistry (Heat Output), Stoichiometry (Ingredients for pyrotechnich mixture), Oxidizer, Fuel, Binder, Ignition, Colour, Black powder, Gun Powder, Effects of Charcoal, Colors and Mixing, Light process, Safety Measures

(30 Lectures)

Reference Books

- Sharma, B. K. Industrial Chemistry (volume 1&2), Krishna Prakashan Media, Meerut (2016).
- Jain, P. C., Jain, M. Engineering Chemistry, Dhanpat Rai & Sons, Delhi (2015).
- Saha, C., Chakraborty, B., Basu, K., Chakraborty, S. Lectures on Pharmaceutical Chemistry and Pesticide Chemistry, Techno World (2020).

- Chopra, H. K., Panesar, P. S. Food Chemistry, Narosa Publishing House, New Delhi (2010).
- Organic Chemistry: Subrata Sen Gupta.
- Organic Chemistry: R.L. Madan.
- Daniel, M., Battacharya, S. D., Arya, A., Raole, V. M. Natural Dyes: Scopes and Challenges

Course Learning Outcomes: After completion of the course, the student should be able to

1. Explain the chemistry of dyes in daily life
2. Familiarize with classification of dyes and chemistry of dyeing process
3. Explore about the application of paints
4. Knowing the various oxidizers used in fireworks industry
5. Significant knowledge in colour producers and safety measures of fireworks

CHEM156MDC03: Elements of Matter and States of Matter

(Credits: 03, Theory:03, 30 Lectures, Full Marks: 50)

Course Objectives: The course aims to provide the basic knowledge on the important discoveries in chemistry and states of matter.

Importance and scope of chemistry

Historical approach to particulate nature of matter, Dalton's atomic theory: concept of elements, atoms, and molecules.

Discovery and the importance of some elements: H, Li, C, O, N, F, Si, P, Fe, As, Au, U

Discovery of electron, proton and neutron; atomic number, isotopes and isobars. Atomic models: qualitative idea

Brief history of the development of periodic table, modern periodic law and the present form of periodic table

States of Matter: Gases and Liquids and Solids

Three states of matter, intermolecular interactions, types of bonding, melting and boiling points.

Gas laws: Boyle's law, Charle's law, Gay Lussac's law, Avogadro's law, ideal gas equation. Kinetic Theory of Gases (elementary idea), deviation from ideal behaviour, liquefaction of gases, critical temperature.

Liquid State – Vapour pressure, viscosity, and surface tension (qualitative idea only, no mathematical derivations).

Classification of solids based on different binding forces: molecular, ionic covalent and metallic solids, amorphous and crystalline solids (elementary idea), unit cell in two dimensional and three-dimensional lattices, Bravais lattice.

(30 Lectures)

Reference Books:

- Jackson, T. Ponderables, The Elements: An Illustrated History of the Periodic Table, Worth Press Limited (2017).
- Castellan, G. W. Physical Chemistry 4th Ed. Narosa (2004).

Course Learning Outcomes: After completion of the course, the student should be able to

1. Demonstrate the landmark discoveries in chemistry
2. Familiarize with the key concepts of chemistry and states of matter

SEMESTER- III

CHEM201C05: ORGANIC CHEMISTRY-II

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Course Objectives: To impart knowledge on the reaction thermodynamics and exploring the chemistry of aliphatic and aryl hydrocarbons, alcohols, phenols, ethers, epoxides, carbonyl compounds, carboxylic acid, and its derivatives.

Chemistry of Aliphatic & Aromatic hydrocarbons and Reaction Thermodynamics

Aliphatic Hydrocarbons (Alkanes, Alkenes, & Alkynes): Preparation and reaction of alkanes (Wurtz, Wurtz-Fittig reactions, Halogenation etc.). Formation of alkenes and alkynes by elimination reactions, Saytzeff and Hofmann eliminations. Reactions of alkenes: Electrophilic additions via Markownikoff and anti-Markownikoff rule, Oxymercuration-demercuration, Hydroboration-oxidation, Ozonolysis, Reduction (catalytic and chemical), *syn-/anti*-hydroxylation (oxidation). 1,2- and 1,4-additions in conjugated dienes, Allylic and Benzylic bromination. Electrophilic and Nucleophilic additions of Alkynes. Acidity of Alkylation of terminal alkynes.

Aromatic Hydrocarbons: Aromaticity, Hückel's rule, Hückel's M.O. theory, Aromatic character of arenes, cyclic carbocations/carbanions and heterocyclic compounds with suitable examples. Electrophilic and Nucleophilic aromatic substitutions: halogenation, nitration, sulphonation, Friedel-Craft's alkylation/acylation, S_NAr, Benzyne mechanism and Directing effects of the groups.

Reaction thermodynamics: Free energy and equilibrium, Enthalpy and Entropy factor, Intermolecular & Intramolecular reactions. Application of thermodynamic principles in tautomeric equilibria, Composition of the equilibrium in different systems such as simple carbonyl, 1,3- and 1,2-dicarbonyl systems, phenols and related system, substituent and solvent effect *etc*. **(18 Lectures)**

Alcohols, Phenols, Ethers and Epoxides

Alcohols: Properties, Preparation from alkenes, and carbonyl compounds, Relative reactivity of 1°, 2°, 3° alcohols, Bouveault-Blanc reduction, Lucas test, Oxidation of alcohols (H_2CrO_4, PDC/PCC, $KMnO_4$, Swern oxidation, DMP, and Oppenauer oxidation).

Glycols: Properties and preparation of glycols (OsO_4, $KMnO_4$, from epoxide, Woodward and Prévost reaction), Oxidation by periodic acid and lead tetraacetate, Pinacol-Pinacolone, semipinacol and Tiffeneau-Demjanov rearrangement.

Phenols: Properties, preparation, acidity, and factors effecting it. Ring substitution reactions: Kolbe–Schmidt Reaction, Reimer–Tiemann formylation, Houben-Hoesch acylation, Dienone-phenol rearrangement, Fries and Claisen rearrangements.

Ethers and Epoxides: Preparations, ether cleavage, and reactions of epoxides with alcohols, ammonia derivatives and LAH. **(14 Lectures)**

Carbonyl Compounds

Preparation of carbonyls – mechanism, equilibrium and kinetic control. Nucleophilic additions: reactions with HCN, bisulfite, Nucleophilic addition-elimination reactions with alcohols, amines, thiols. Reaction with ylides: Wittig and Corey-Chaykovsky reaction. Benzoin condensation, Cannizzaro, and Benzil-Benzilic acid rearrangements. Baeyer-Villiger oxidation, α-substitution reactions, oxidations, reductions (Clemmensen, Wolff-Kishner, LAH, $NaBH_4$, MPV, PDC and PCC). Active methylene compounds: Keto-enol tautomerism. Preparation and synthetic applications of diethyl malonate and ethyl acetoacetate.

Formation of enols and enolates, kinetic and thermodynamic enolates, Haloform reaction. Condensation reactions: Aldol and Knoevenagel condensation, Claisen-Schmidt, Perkin, Stobbe, and Mannich reactions. Addition to α,β-unsaturated carbonyls: Direct and conjugate addition, Michael addition, Robinson annulations. **(14 Lectures)**

Carboxylic acids with derivatives and Organometallics

Preparation, and reactions of monocarboxylic acids. Typical reactions of dicarboxylic acids, hydroxy acids, and unsaturated acids. Preparation and reactions of acid chlorides, anhydrides, esters and amides. Comparative study of nucleophilic substitution of acyl group – Mechanism of acidic and alkaline hydrolysis of esters, Claisen condensation, Dieckmann, Reformatsky, and Beckmann reactions, Hofmann bromamide degradation and Curtius rearrangement.

Organometallic compounds of Mg and Li – Use in synthesis of organic compounds.

(14 Lectures)

Reference Books:

- Finar, I. L. *Organic Chemistry (Vol. I)*, 6th Ed., Pearson (2002).
- Graham Solomons, T. W.; Fryhle, C. B. & Snyder, S. A. *Organic Chemistry,* 12th Ed., John Wiley & Sons (2017).
- Clayden, J.; Greeves, N. & Warren, S. *Organic Chemistry*, 2nd Ed., Oxford University Press (2012).

- Sykes, P. *A Guidebook to Mechanism in Organic Chemistry,* Orient Longman, New Delhi (1988).
- Smith, M. B. *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, 8th Ed., Wiley (2020).
- McMurry, J. E. *Fundamentals of Organic Chemistry*, 7th Ed., Cengage Learning India Edition (2013).

CHEMISTRY PRACTICAL – CHEM201C05 LAB

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

1. Purification of organic liquids by distillation and determination of the boiling point.

2. Organic Preparations:

(i) Oxidation of ethanol/isopropanol (Iodoform reaction).

(ii) Bromination of acetanilide by conventional methods or green approach (Bromate-bromide method).

(iii) Nitration of any one of the following:

(a) Acetanilide/nitrobenzene by conventional method.

(b) Salicylic acid by green approach (using ceric ammonium nitrate).

(iv) Selective reduction of *m*-dinitrobenzene to *m*-nitroaniline.

(v) Reduction of *p*-nitrobenzaldehyde by $NaBH_4$.

(vi) Hydrolysis of amides and esters.

(vii) Aldol condensation using either conventional or green method.

(viii) Benzil-Benzilic acid rearrangement.

Reference Books:

- Mann, F. G. & Saunders, B. C. *Practical Organic Chemistry*, Pearson (2009).
- Furniss, B. S.; Hannaford, A. J.; Smith, P. W. G. & Tatchell, A. R. *Vogel's Textbook of Practical Organic Chemistry*, 5th Ed., Pearson (2012).
- Ahluwalia, V. K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis*, University Press (2000).
- Ahluwalia, V. K. & Dhingra, S. *Comprehensive Practical Organic Chemistry: Qualitative Analysis*, University Press (2000).

Course Learning Outcomes: After completion of the course, the student should be able to

1. Predict aromatic, anti-aromatic and non-aromatic characters of cyclic, conjugated polyenes via MOT and apply this concept to rationalize the reactions of aromatic species with various electrophiles and nucleophiles.

2. Analyse several physical parameters controlling the organic transformations and comprehend the chemistry of numerous functionalized organic compounds.
3. Prepare different organic derivatives utilizing one step reaction.

CHEM202C06: PHYSICAL CHEMISTRY- II

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Course Objectives: To impart knowledge on the application of classical thermodynamics and to build concepts on the solution properties, reaction kinetics, surface phenomena.

Chemical Equilibrium:

Criteria of thermodynamic equilibrium, degree of advancement of reaction, chemical equilibria in ideal gases, concept of fugacity. Thermodynamic derivation of relation between Gibbs free energy of reaction and reaction quotient. Coupling of exoergic and endoergic reactions. Equilibrium constants and their quantitative dependence on temperature, pressure and concentration. Free energy of mixing and spontaneity; thermodynamic derivation of relations between the various equilibrium constants *Kp*, *Kc* and *Kx*. Le Chatelier principle (quantitative treatment); equilibrium between ideal gases and a pure condensed phase.

(6 Lectures)

Solutions and Colligative Properties:

Dilute solutions; lowering of vapour pressure, Raoult's and Henry's Laws and their applications.

Thermodynamic derivation using chemical potential to derive relations between the four colligative properties [(i) relative lowering of vapour pressure, (ii) elevation of boiling point, (iii) Depression of freezing point, (iv) osmotic pressure] and amount of solute. Applications in calculating molar masses of normal, dissociated and associated solutes in solution.

(8 Lectures)

Chemical Kinetics

Phenomenological kinetics: degree of advancement of a reaction, reaction rate, rate constant, order and molecularity of a reaction, rate laws in terms of the advancement of a reaction, differential and integrated form of rate expressions up to second order reactions, experimental methods of the determination of rate laws, kinetics of complex reactions (integrated rate expressions up to first order only): (i) Opposing reactions (ii) parallel reactions and (iii) consecutive reactions and their differential rate equations (steady-state approximation in reaction mechanisms) (iv) chain reactions. Differential rate law for complex reactions following reaction mechanism.

Temperature dependence of reaction rates; Arrhenius equation; activation energy. Collision theory of reaction rates, Lindemann mechanism, Collision theory: Introduction of potential

energy surface and contour, internal coordinates and reaction coordinates, reaction path – valley and saddle point; saddle point – activation energy, classical trajectory, and theory of absolute rate. Comparison of collision and absolute rate theory, primary and secondary kinetic salt effect, kinetic isotope effect.

(20 Lectures)

Catalysis

Types of catalyst, specificity and selectivity, mechanisms of catalyzed reactions at solid surfaces; effect of particle size and efficiency of nanoparticles as catalysts. Enzyme catalysis, Michaelis-Menten mechanism, turnover number, Lineweaver-Burk plot; influence of temperature and pH, Acid-base catalysis. Heterogeneous catalysis (single reactant).

(**6 Lectures)**

Surface Phenomena

Surface tension, surface energy (thermodynamic treatment), excess pressure, capillary rise and measurement of surface tension, work of cohesion and adhesion, spreading of liquid over other surface, vapour pressure over curved surface, temperature dependence of surface tension. Effect of addition of various solutes on surface tension. Physical adsorption, chemisorption, adsorption isotherms. nature of adsorbed state. Freundlich and Langmuir adsorption isotherm, isosteric heat of adsorption, multilayer and BET isotherm and applications, feasibility of adsorption process, Gibbs adsorption isotherm and surface excess, surface film, properties of very small particles.

(20 Lectures)

Reference Books

- Peter, A. & Paula, J. de. Physical Chemistry 10th Ed., Oxford University Press (2014).
- Castellan, G. W. Physical Chemistry 4th Ed., Narosa (2004).
- Engel, T. & Reid, P. Physical Chemistry 3rd Ed., Prentice-Hall (2012).
- McQuarrie, D. A. & Simon, J. D. Molecular Thermodynamics Viva Books Pvt. Ltd.:New Delhi (2004).
- Assael, M. J.; Goodwin, A. R. H.; Stamatoudis, M.; Wakeham, W. A. & Will, S. Commonly Asked Questions in Thermodynamics. CRC Press: NY (2011).
- Levine, I .N. Physical Chemistry 6th Ed., Tata Mc Graw Hill (2010).
- Metz, C.R. 2000 solved problems in chemistry, Schaum Series (2006).

CHEMISTRY PRACTICAL – CHEM202C06 LAB

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

1. Study the kinetics of the following reactions

(i) Initial rate method:

a. Iodide-persulphate reaction

(ii) Integrated rate method:

a. Acid hydrolysis of methyl acetate with hydrochloric acid.

b. Saponification of ethyl acetate.

2. Adsorption

Verification of the Freundlich isotherms for adsorption of acetic acid on activated charcoal.

3. Surface tension measurements

(i) Determine the surface tension.

(ii) Study the variation of surface tension of detergent solutions with concentration.

Reference Books

- Khosla, B. D.; Garg, V. C. & Gulati, A., Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011).
- Athawale, V. D. & Mathur, P. Experimental Physical Chemistry New Age International: New Delhi (2001).

Course Learning Outcomes: After the completion of the course, the students should be able to

1. Explain the origin of equilibrium constant and its relation to fugacity and activity and apply these concepts to ideal and real solutions of electrolytes and non-electrolytes and to colligative properties.
2. List the methods for arriving at rate law based on kinetic information.
3. Apply the steady-state hypothesis to obtain rate equations and explain the effect of temperature, addition of salt, isotopic substitution and catalyst on the rate constant.
4. Demonstrate the various surface phenomena, such as surface tension, adsorption and explain the effect of temperature, addition of various solutes and surfactants on the surface tension.

CHEM241SEC01.1: IT SKILLS FOR CHEMISTS

(Credits: 04, 60 Lectures, Full Marks: 50)

Course Objectives: To acquire mathematical and computational skills that can be applied on the relevant research areas.

Mathematics:

Fundamentals, mathematical functions, polynomial expressions, logarithms, the exponential function, units of a measurement, interconversion of units, constants and variables, equation of a straight line, plotting graphs.

Uncertainty in experimental techniques: Displaying uncertainties, measurements in chemistry, decimal places, significant figures, combining quantities.

Uncertainty in measurement: types of uncertainties, combining uncertainties. Statistical treatment. Mean, standard deviation, relative error. Data reduction and the propagation of errors. Graphical and numerical data reduction. Numerical curve fitting: the method of least squares (regression).

Algebraic operations on real scalar variables (e.g. manipulation of van der Waals equation in different forms). Roots of quadratic equations analytically and iteratively (e.g. pH of a weak acid). Numerical methods of finding roots (Newton-Raphson, binary –bisection, e.g. pH of a weak acid not ignoring the ionization of water, volume of a van der Waals gas, equilibrium constant expressions).

Differential calculus: The tangent line and the derivative of a function, numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations).

Numerical integration (Trapezoidal and Simpson's rule, e.g. entropy/enthalpy change from heat capacity data).

Numerical solution of first order ordinary differential equation. Euler's method and improved Euler method.

Computer programming:

Constants, variables, bits, bytes, binary and ASCII formats, arithmetic expressions, hierarchy of operations, inbuilt functions. Elements of the BASIC language (FORTRAN). BASIC keywords and commands. Logical and relative operators. Strings and graphics. Compiled versus interpreted languages. Debugging. Simple programs using these concepts. Matrix addition and multiplication. Statistical analysis.

BASIC programs for curve fitting, numerical differentiation, and integration (Trapezoidal rule, Simpson's rule), finding roots (quadratic formula, iterative, Newton-Raphson method), numerical solution of first order differential equation: Euler's method, predictor-corrector method.

HANDS ON

Introductory writing activities: Introduction to word processor and structure drawing (Chem Sketch) software. Incorporating chemical structures, chemical equations, expressions from chemistry (e.g., Maxwell-Boltzmann distribution law, Bragg's law, van der Waals equation, etc.) into word processing documents.

Introduction to LATEX: Writing articles, equations, making tables, inserting figures and references.

Handling numeric data: Spreadsheet software (Excel/Origin/Gnuplot), creating a spreadsheet, entering, and formatting information, basic functions and formulae, creating charts, tables and graphs.

Incorporating tables and graphs into word processing documents. Simple calculations, plotting graphs using a spreadsheet (Planck's distribution law, radial distribution curves for hydrogenic orbitals, gas kinetic theory- Maxwell-Boltzmann distribution curves as function of temperature and molecular weight), spectral data, pressure-volume curves of van der Waals gas (van der Waals isotherms), data from phase equilibria studies. Graphical solution of equations.

Numeric modelling: Simulation of pH metric titration curves. Excel functions LINEST and Least Squares. Numerical curve fitting (Origin), linear regression (rate constants from concentration time

data, molar extinction coefficients from absorbance data), numerical differentiation (e.g., handling data from potentiometric and pH metric titrations, pKa of weak acid), integration (e.g., entropy/enthalpy change from heat capacity data).

Symbolic Computation:

Symbolic computation of simple algebra and numerical mathematics using Mathematica/Matlab software: Plotting mathematical functions, solving algebraic equations, differentiation, integration, integral transform, series, solving differential equations, performing matrix algebra, curve fitting.

Statistical analysis: Gaussian distribution and Errors in measurements and their effect on data sets. Descriptive statistics using Excel.

Presentation: Presentation graphics (Power Point Presentation).

Reference Books:

- McQuarrie, D. A. *Mathematics for Physical Chemistry University* Science Books (2008).
- Mortimer, R. *Mathematics for Physical Chemistry*. 3rd Ed. Elsevier (2005).
- Steiner, E. *The Chemical Maths Book* Oxford University Press (1996).
- Yates, P. *Chemical calculations.* 2nd Ed. CRC Press (2007).
- Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007) Chapters 3-5.
- Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis*, Cambridge Univ. Press (2001) 487 pages.
- Noggle, J. H. *Physical chemistry on a Microcomputer.* Little Brown & Co. (1985).
- Venit, S.M. *Programming in BASIC: Problem solving with structure and style*. Jaico Publishing House: Delhi (1996).

Course Learning Outcomes: After the completion of the course, the students should be able to

1. Formulate a set of calculations that can address a relevant research question.
2. Use one or several computer programs and extract useful information.
3. Write a research paper that describes methods, results, and interpretation.
4. Assess the meaning and validity of calculations that appear in the chemical literature.

Skill Enhancement Course (Credit: 04 each)
CHEM241SEC01.2: Quality Control Analysis of Commercial Products

(Credits: 04, 60 Lectures, Full Marks: 50)

Course Objectives: The course aims to provide the student's hands-on training on various advanced analytical methods involved in the chemical analysis of commercial products used in day-to-day life.

Volumetric analysis: Principles of quantitative analysis by volumetric titrations, Equivalence point & End point, Direct & Back titrations, Indicators, pH metric titrations, Permanganometry, Zimmermann and Reinhardt's solution, Dichromatometry, Iodine titration, Complexometric titrations, Stability constant, Masking & Demasking reactions, Limitations & Detection levels of volumetric analysis

Advanced spectroscopic methods for quantitative analysis: Lambert Beer Law, Atomic Absorption Spectroscopy, Atomic Emission Spectroscopy, Flame Photometry, Elementary theory, Method of quantitative estimations, Basic instrumentations: Flame, Line source, Hollow cathode lamp, Monochromator, Detector, Limitations & Detection levels of spectroscopic methods for quantitative analysis

Hands on experience on the following experiments (Any Five)

1. Estimation of available chlorine from bleaching powder
2. Estimation of the amount of calcium in milk powder
3. Estimation of phosphoric acid in cola drinks
4. Estimation of iodine in iodized common salt
5. Estimation of free alkali present in different soaps/detergents
6. Estimation of total manganese from pyrolusite
7. Estimation of copper in brass
8. Determination of hardness of water

Reference Books:

- A. J. Elias, A Collection of Interesting General Chemistry Experiments, Sangam Books
- R. L. Madan, Chemistry: for B.Sc. Students, S. Chand Publishing, 2020
- G. N. Mukherjee, Advanced Experiments in Inorganic Chemistry, U. N. Dhur & Sons(p) ltd.
- Willard, H.H., Merritt, L.L., Dean, J. &Settoe, F.A. *Instrumental Methods of Analysis*, 7th Ed. Wadsworth Publishing Company Ltd., Belmont, California, USA,1988.
- Skoog, D.A., Holler, F.J. & Crouch, S. *Principles of Instrumental Analysis*, Cengage Learning India Edition, 2007.

- Skoog, D.A.; West, D.M. & Holler, F.J. *Analytical Chemistry: An Introduction 6th Ed.,* Saunders College Publishing, Fort Worth, Philadelphia (1994).
- Harris, D. C. *Quantitative Chemical Analysis*, 9th ed. Macmillan Education, 2016.
- Dean, J. A. *Analytical Chemistry Handbook*, McGraw Hill, 2004.

Course Learning Outcomes: Upon completion of the course, the students should be able to analyze all the day-to-day commercial samples qualitatively, and quantitatively using traditional and advanced techniques.

CHEM205MC03

Theory: Solutions, Phase Equilibria, Conductance, Electrochemistry & Functional Group Organic Chemistry

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Section A: Physical Chemistry

Course Objectives: To impart knowledge on the application of classical thermodynamics on phase, solutions and build basic concepts of conductance and electrochemistry.

Solutions

Thermodynamics of ideal solutions, Ideal solutions and Raoult's law, deviations from Raoult's law–non-ideal solutions. Vapour pressure-composition and temperature-composition curves of ideal and non-ideal solutions, Distillation of solutions, Lever rule, Partial miscibility of liquids, Critical solution temperature, effect of impurity on partial miscibility of liquids, Nernst distribution law and its applications, solvent extraction. **(8 Lectures)**

Phase Equilibria

Phases, Components and degrees of freedom of a system, criteria of phase equilibrium. Gibbs phase rule and its thermodynamic derivation, Derivation of Clausius-Clapeyron equation and its importance in phase equilibria. Phase diagrams of one-component systems (water and sulphur) and two component systems involving eutectics. **(8 Lectures)**

Conductance

Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Kohlrausch law of independent migration of ions. Transference number and its experimental determination using Hittorf and Moving boundary methods. Ionic mobility, Applications of conductance measurements, determination of degree of ionization of weak electrolyte, solubility and solubility products of sparingly soluble salts, ionic product of water, hydrolysis constant of a salt. Conductometric titrations (only acid base). **(6 Lectures)**

Electrochemistry

Reversible and irreversible cells, Concept and measurement of EMF of a cell, Nernst equation and its importance, Types of electrodes, Standard electrode potential, Electrochemical series. Thermodynamics of a reversible cell, calculation of thermodynamic properties: ΔG, ΔH and ΔS from EMF data. Calculation of equilibrium constant from EMF data. Concentration cells with and without transference, Liquid junction potential and salt bridge, pH determination using hydrogen electrode and quinhydrone electrode. Potentiometric titrations qualitative treatment (acid-base and oxidation-reduction only).

(8 Lectures)

Section B: Organic Chemistry

Course Objectives: To impart knowledge on the chemistry of carboxylic acids, amines, diazonium salts, amino acids, peptides, proteins, and carbohydrates.

Carboxylic acids and their derivatives

Carboxylic acids (aliphatic and aromatic) – Preparation, acidic and alkaline hydrolysis of esters, Hell-Volhard-Zelinsky reaction, Preparation of acid chlorides, anhydrides, esters and amides from acids and their interconversion. Comparative study of electrophilicity of acyl derivatives, Reformatsky reaction, Perkin condensation. **(6 Lectures)**

Amines and Diazonium Salts

Amines (Aliphatic and Aromatic, upto 5 carbons): Preparation from alkyl halides, Gabriel Phthalimide synthesis, Hofmann Bromo amide reaction (Hofmann Degradation). Hofmann vs. Saytzeff elimination, Carbylamine test, Hinsberg test, reaction with HNO_2, Schötten-Baümann Reaction. Electrophilic substitution (aniline) – nitration, bromination, sulphonation.

Diazonium salts: Preparation from aromatic amines, conversion to benzene, phenol, and dyes. **(6 Lectures)**

Amino Acids, Peptides and Proteins

Preparation of amino acids by Strecker and Gabriel phthalimide synthesis. Zwitterion, Isoelectric point and Electrophoresis. Reactions of amino acids: esterification, of $–CO_2H$,

acetylation of $-NH_2$, complexation, ninhydrin test. Overview of primary, secondary, tertiary and quaternary structures of proteins, Determination of primary structure of peptides by degradation – Edmann degradation (N-terminal), with thiohydantoin and carboxypeptidase enzyme (C-terminal). Synthesis of simple peptides (upto dipeptides) by N-protection (*t*-butyloxycarbonyl and phthaloyl) and C-activating groups and Merrifield solid-phase synthesis. **(10 Lectures)**

Carbohydrates

Classification, general properties, Glucose and Fructose (open chain and cyclic structure), Determination of configuration of monosaccharides, absolute configuration of Glucose and Fructose, Mutarotation, ascending and descending in monosaccharides. Structure of disaccharides (sucrose, cellobiose, maltose, lactose) and polysaccharides (starch and cellulose) excluding their structure elucidation. **(8 Lectures)**

Reference Books:

- Barrow, G. M. *Physical Chemistry,* Tata McGraw-Hill (2007).
- Castellan, G. W. *Physical Chemistry,* 4th Ed., Narosa (2004).
- Kotz, J. C.; Treichel, P. M. & Townsend, J. R. *General Chemistry*, Cengage Learning India Pvt. Ltd.: New Delhi (2009).
- Mahan, B. H. *University Chemistry*, 3rd Ed., Narosa (1998).
- Petrucci, R. H. *General Chemistry*, 5th Ed., Macmillan Publishing Co.: New York (1985).
- Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, 7th Ed., Pearson Education India (2011).
- Finar, I. L. *Organic Chemistry (Vol. I)*, 6th Ed., Pearson (2002).
- Finar, I. L. *Organic Chemistry* (*Vol. II)*, Pearson (2002).
- Nelson, D. L. & Cox, M. M. *Lehninger's Principles of Biochemistry*, 7th Ed., W. H. Freeman & Co. (2017).
- Berg, J. M.; Tymoczko, J. L. & Stryer, L. *Biochemistry*, W. H. Freeman & Co. (2002).

CHEM205MC03 Lab: (Credits: 02, 60 Lectures, Full Marks: 30)

Section A: Physical Chemistry

Distribution

Study of the equilibrium of one of the following reactions by the distribution method:

$I_2(aq) + I(aq) = I_3^-(aq)$

$Cu^{2+}(aq) + xNH_3(aq) = [Cu(NH_3)_x]^{2+}$

Phase equilibria

Determination of the critical solution temperature and composition of the phenol water system and study of the effect of impurities on it.

Conductance

1. Determination of cell constant.

2. Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid.

3. Perform the following conductometric titrations:

(a) Strong acid vs. strong base

(b) Weak acid vs. strong base

Potentiometry

1. Perform the following potentiometric titrations (*any two*):

(a) Strong acid vs. strong base

(b) Weak acid vs. strong base

(c) Potassium dichromate vs. Mohr's salt

Section B: Organic Chemistry

1. Systematic qualitative analysis of organic compounds bearing nitrogenous and non-nitrogenous functional groups and preparation of one derivative.

2. Separation of amino acids by paper chromatography.

3. Determination of the concentration of glycine solution by formylation method.

4. Titration curve of glycine.

5. Action of salivary amylase on starch.

6. Effect of temperature on the action of salivary amylase on starch.

7. Differentiation between a reducing and a nonreducing sugar.

Reference Books:

- Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry,* R. Chand & Co.: New Delhi (2011).
- Vogel, A. I.; Tatchell, A. R.; Furnis, B. S.; Hannaford, A. J. & Smith, P.W.G. *Textbook of Practical Organic Chemistry*, 5th Ed., Prentice-Hall (1996).
- Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry* Orient-Longman (1960).
- Ahluwalia, V. K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry,* Universities Press (2004).

Course Learning Outcomes: After completion of the course, the student should be able to

1. Interpret phase diagrams and explain phase equilibria in terms of chemical potentials.
2. Calculate the degrees of freedom for various types of systems
3. Explain how phase equilibria aid in understanding the formation of various materials, allotropic forms of different substances and the formation of binary mixtures, azeotropes.
4. Apply the principles of electrochemistry to conductance, voltaic, and electrolytic systems.
5. Comprehend the reactivity of acyl carbon toward different nucleophiles.
6. Conduct synthesis, separation, and identification of 1°, 2°, and 3°-amines and their reactions.
7. Elucidate primary, secondary, tertiary and quaternary structures of proteins; determine structure of peptides and carry out synthesis and reactions of amino acids.
8. Explain physical, chemical and optical properties of basic units of carbohydrates.
9. Detect nitrogenous and non-nitrogenous functional groups and separation of organic molecules.

SEMESTER- IV

CHEM251C07: INORGANIC CHEMISTRY-III

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Course Objectives: The course aims to provide the knowledge on advanced theories of coordination compounds and their applications. Introduce the concept of nuclear chemistry and chemical elements in life. Weak chemical forces. Acid –base theory of Inorganic compounds. Qualitative inorganic salt analysis.

Electronic Spectra and Magnetism:

Ligand field and MO Theory. Orgel diagrams for $3d^{l}$-$3d^{9}$ ions and their spectroscopic ground states; selection rules for electronic spectral transitions; spectrochemical series of ligands; d-d transitions, L-S coupling, charge transfer spectra (LMCT & MLCT). Definition of magnetic properties, types of magnetic bodies, Curie equation, Curie's law and Curie-Weiss law. Orbital and spin magnetic moments, spin only moments of d^{n} ions and their correlation with effective magnetic moments, including orbital contribution; quenching of magnetic moment: super exchange and ferromagnetic/antiferromagnetic interactions. Lande interval rule, energies of J levels. Spin state isomerization, spin-crossover, magnetic behavior of lanthanides and actinides, magnetic exchange interactions. **(18 Lectures)**

Nuclear Chemistry:

Classification of nuclides based on the number of nucleons- Isotopes, Isobars, Isotones; Nuclear Isomer and isomeric transition; Radius and Density of Nucleus; Nuclear Spin; Shape of Nucleus; Nuclear Stability; The Neutron to Proton Ratio and Different Modes of Decay; Fajans & Soddy's Group Displacement Law; Artificial Radioactivity; Nuclear Reactions; Nuclear Reaction Cross-Section; The Disintegration Series; Packing Fraction, Nuclear Binding Energy and Nuclear Stability; Radioactive Decay Kinetics; Application of Radioactivity in Age Determination; Nuclear Forces; Nuclear Models-Fermi Gas Model, Liquid Drop Model, Nuclear and Shell Model **(13 Lectures)**

Weak Chemical Forces: van der Waals forces, ion-dipole forces, dipole-dipole interactions, induced dipole interactions, Instantaneous dipole-induced dipole interactions. Repulsive forces, Hydrogen bonding (theories of hydrogen bonding, valence bond treatment) Effects of chemical force, melting and boiling points. **(6 Lectures)**

Bioinorganic Chemistry-1:

Elements of life: essential, major, trace and ultratrace elements. Basic chemical reactions in the biological systems and the role of metal ions (specially Na^+, K^+, Mg^{2+}, Ca^{2+}, $Fe^{3+/2+}$,$Cu^{2+/+}$, and Zn^{2+}). Ionophores, Sodium potassium pump. Biological functions of hemoglobin and myoglobin, cytochromes and ferredoxins. **(8 Lectures)**

Acids and Bases:

Bronsted and Lowry's concept, solvent system concept, Lewis concept, Lux-Flood concept, relative strength of acids, hydracids and oxyacids, Pauling's rules, amphoterism, and super acids, HSAB principle, acid-base equilibria in aqueous solution, pH, buffer solutions and buffer actions, acid-base neutralization curves, acid-base indicators, choice of indicators, acid-base titrations. **(12 Lectures)**

Non-aqueous Solvents:

Physical properties of a solvent, types of solvents and their general characteristics, reactions in non-aqueous solvents such as HF, H_2SO_4, NH_3, CH_3COOH, etc… **(3 Lectures)**

Reference Books:

- W. U. Malik, G. D. Tuli, R. D. Madan, Selected Topics in Inorganic Chemistry, S. Chand Publishers, 2001
- R. L. Dutta & G.S. De, Inorganic Chemistry (Vol. 1), The New Book Stall, 1973.
- Purcell, K.F & Kotz, J.C. Inorganic Chemistry W.B. Saunders Co, 1977.
- Huheey, J. E.; Keiter, E.A. & Keiter, R.L. Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed., Harper Collins 1993, Pearson,2006.
- Essentials of Nuclear Chemistry by H. J. Arnikar
- Lippard, S.J. & Berg, J.M. Principles of Bioinorganic Chemistry Panima Publishing Company 1994.
- Cotton, F.A. & Wilkinson, G, Advanced Inorganic Chemistry Wiley-VCH, 1999
- Asim K Das, Bioinorganic Chemistry
- Asim K. Das, Fundamental Concepts of Inorganic Chemistry, **CBS Publishers &Distributors** Pvt Ltd ed. 2, Vol. 3, 2019.
- R. D. Madan, Modern Inorganic Chemistry, **S. CHAND & COMPANY LTD.,** 3rd revised Ed., 2011
- David W. Oxtoby, H.P. Gillis, Alan Campion, Principles Of Modern Chemistry, 7th Ed., Cengage Learning, 2012

Inorganic Qualitative Analysis - 1 CHEM251C07 LAB

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

Cation radicals derived from:

Na, K, NH_3, Mg, Ca, Sr, Ba, Al, Pb, Cr, Mn, Fe, Co, Ni, Cu, Zn

Anion radicals:

F^-, CI^-, Br^-, I^-, NO_3^-, NO_2^-, SCN^-, S^{2-}, SO_4^{2-}, $S_2O_3^{2-}$, PO_4^{3-}, BO_3^{3-}, CrO_4^{2-}

Detection of four radicals by macro, semi- micro tests.

Reference Books

- Vogel's Qualitative Inorganic Analysis, Revised by G. Svehla. Pearson Education, 2002.
- G. N. Mukherjee, Hand Book of Inorganic Analysis, U. N. Dhar & sons (P) LTD, 2014
- Marr & Rockett Practical Inorganic Chemistry. John Wiley & Sons 1972.

Course Learning Outcomes: On completion of the course, the students should be able to

1. Explain the structure, spectral and magnetic properties of coordination complexes
2. Predict spectral properties using various theory of coordination chemistry
3. Familiar with elementary idea of nuclear chemistry, nuclear reactions and kinetics
4. Acquire the knowledge on weak chemical forces and their applications
5. Explain functioning of important enzymes and proteins in our body
6. Acid base property, hard soft acid base etc are taught. pH calculation of solutions, buffers, indicators are taught which have good **industrial applications.**
7. Know the theoretical and practical knowledge on separation and analysis of individual inorganic cations and anions using chemical principles
8. Unravel the various weak inter- & intra molecular forces involved in chemical bonds

CHEM252C08: PHYSICAL CHEMISTRY-III

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Course Objectives: To impart knowledge on the application of classical thermodynamics on phase and ionic equilibria and build basic concepts of electrochemistry.

Phase Equilibria:

Concept of phases, components and degrees of freedom, derivation of Gibbs Phase Rule for nonreactive and reactive systems; Clausius-Clapeyron equation and its applications to solid liquid, liquid-vapour and solid-vapour equilibria, phase diagram for one component systems, with applications.

Phase diagrams for systems of solid-liquid equilibria involving eutectic, congruent and incongruent melting points, solid solutions.

Three component systems, water-chloroform-acetic acid system, triangular plots.

Binary solutions: Gibbs-Duhem-Margules equation, its derivation and applications to fractional distillation of binary miscible liquids (ideal and nonideal), azeotropes, lever rule, partial miscibility of liquids, CST, miscible pairs, steam distillation.

Nernst distribution law: its derivation and applications: solvent extraction, determination of equilibrium constant.

(26 Lectures)

Ionic equilibria:

Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale; dissociation constants of mono-, di-and triprotic acids (exact treatment).

Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions; derivation of Henderson equation and its applications; buffer capacity, buffer range, buffer action and applications of buffers in analytical chemistry and biochemical processes in the human body.

Solubility and solubility product of sparingly soluble salts – applications of solubility product principle. Qualitative treatment of acid – base titration curves (calculation of pH at various stages). Theory of acid–base indicators; selection of indicators and their limitations.

(14 Lectures)

Electrochemistry-I

Quantitative aspects of Faraday's laws of electrolysis, rules of oxidation/reduction of ions based on half-cell potentials, applications of electrolysis in metallurgy and industry. Chemical

cells, reversible and irreversible cells with examples. Electromotive force of a cell and its measurement, Nernst equation; Standard electrode (reduction) potential and its application to different kinds of half-cells. Application of EMF measurements in determining

(i) free energy, enthalpy and entropy of a cell reaction, (ii) equilibrium constants, and (iii) pH values, using hydrogen, quinone-hydroquinone, glass and SbO/Sb_2O_3 electrodes.

Concentration cells with and without transference, liquid junction potential; determination of activity coefficients and transference numbers. Qualitative discussion of potentiometric titrations (acid-base, redox, precipitation).

(20 Lectures)

Reference Books:

- Peter Atkins & Julio De Paula, Physical Chemistry 10th Ed., Oxford University Press (2014).
- Castellan, G. W. Physical Chemistry, 4th Ed., Narosa (2004).
- McQuarrie, D. A. & Simon, J. D., Molecular Thermodynamics, Viva Books Pvt. Ltd.: New Delhi (2004).
- Engel, T. & Reid, P. Physical Chemistry 3rd Ed., Prentice-Hall (2012).
- Assael, M. J.; Goodwin, A. R. H.; Stamatoudis, M.; Wakeham, W. A. & Will, S. Commonly Asked Questions in Thermodynamics. CRC Press: NY (2011).
- Zundhal, S.S. Chemistry concepts and applications Cengage India (2011).
- Ball, D. W. Physical Chemistry Cengage India (2012).
- Mortimer, R. G. Physical Chemistry 3rd Ed., Elsevier: NOIDA, UP (2009).
- Levine, I. N. Physical Chemistry 6th Ed., Tata McGraw-Hill (2011).
- Metz, C. R. Physical Chemistry 2nd Ed., Tata McGraw-Hill (2009).
- Glasstone, S. An Introduction to Electrochemistry, Affiliated East-West Press Private Limited (2003).
- Bockris, J.O'M., Reddy, A.K.N., Modern Electrochemistry 1, 2nd Ed., Springer (2012)

CHEMISTRY PRACTICAL- CHEM252C08 LAB

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

1. Determination of critical solution temperature and composition of the phenol-water system and to study the effect of impurities on it.
2. Distribution of acetic/ benzoic acid between water and cyclohexane.
3. Study the equilibrium of at least one of the following reactions by the distribution method:

   (a) $I_2\,(aq) + I^- \rightarrow I_3^-\,(aq)$ (ii) $Cu^{2+}\,(aq) + n NH_3 \rightarrow Cu(NH_3)n$

4. **Potentiometry**

   Perform the following potentiometric titrations:

(i) Strong acid vs. strong base

(ii) Weak acid vs. strong base

(iii) Dibasic acid vs. strong base

(iv) Potassium dichromate vs. Mohr's salt

(v) Determination of standard reduction potential of quinhydrone electrode.

(vi) Potentiometric determination of strength of halide mixture.

Reference Books:

- Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011).
- Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry 8th Ed.; McGraw-Hill: New York (2003).
- Halpern, A. M. & McBane, G. C. Experimental Physical Chemistry 3rd Ed.; W.H. Freeman & Co.: New York (2003).

Course Learning Outcomes: After the completion of the course, the students should be able to

1. Interpret phase diagrams and explain phase equilibria in terms of chemical potentials.
2. Calculate the degrees of freedom for various types of systems
3. Explain how phase equilibria help in understanding the formation of various materials, allotropic forms of different substances and the formation of binary mixtures, azeotropes.
4. Explain the use of electrical energy for initiating chemical reactions and also how chemical reactions can be utilized to produce electrical energy, and the basic principle used in the formation of cells and batteries.
5. Perform potentiometric and pH-metric titrations and prepare various buffer solutions.

CHEM291SEC02.1: Pharmaceutical Chemistry & Chemistry of Non-covalent Compounds

(Credits: 05, 60 Lectures, Full Marks: 50)

Course Objectives: To impart knowledge on the theories of drugs, pharmaceuticals, supramolecules, and fermentation processes.

Drugs & Pharmaceuticals

Discovery, design and development of drugs, Basic Retrosynthetic approach, Synthesis of some representative drugs of the following classes – Analgesics, Antipyretic, Anti-inflammatory (aspirin, paracetamol, ibuprofen), Antibiotics (chloramphenicol), and Antimalarials (chloroquine). Medicinal values of curcumin (haldi), azadirachtin (neem), and antacid (ranitidine). Antibacterial and antifungal agents (sulphonamides, sulphanethoxazol, sulphacetamide, and trimethoprim), Antiviral agents (acyclovir), Central Nervous System agents (phenobarbital, diazepam), Cardiovascular (glyceryl trinitrate), Anti-leprosy (dapsone), HIV-AIDS related drugs (AZT- Zidovudine).

Fermentation

Aerobic and anaerobic fermentation. Production of (i) Ethyl alcohol and citric acid, (ii) Antibiotics, Penicillin, Cephalosporin, Chloromycetin and Streptomycin, (iii) Lysine, Glutamic acid, Vitamin B2, Vitamin B12 and Vitamin C.

Chemistry of Non-covalent Compounds

Selectivity, Host-Guest interactions, Molecular wire, Threading-Unthreading, Molecular switches.

Practical

1. Preparation of Aspirin and its analysis.
2. Preparation of magnesium bisilicate (Antacid).

Reference Books:

- Patrick, G. L. *Introduction to Medicinal Chemistry,* Oxford University Press (2013).
- Singh, H. & Kapoor, V. K. *Medicinal and Pharmaceutical Chemistry,* Vallabh Prakashan (2012).

- Foye, W. O.; Lemke, T. L. & William, D. A. *Principles of Medicinal Chemistry*, 6th Ed., Lippincott Williams & Wilkins, Philadelphia (2008).
- Lehn, J-M. *Supramolecular Chemistry - Concepts and Perspectives*, Wiley-VCH Verlag GmbH (1995).

Course Learning Outcomes: After completion of this course students should be able to

1. Design and develop synthetic routes to access various organic compounds with analgesics, antipyretic, anti-inflammatory, antibiotic, antibacterial, antifungal, antiviral and other significant pharmacological activities.
2. Explain aerobic and anaerobic fermentation and their roles in the production of ethanol and citric acid.
3. Conduct synthesis and reactions of important antibiotics such as, Penicillin, Cephalosporin, Chloromycetin and Streptomycin.
4. Describe the pharmaceutical activities of Lysine, Glutamic acid, Vitamin B2, Vitamin B12 and Vitamin C.
5. Synthesize simple and small drug molecules.
6. Understand many biological processes that rely structurally and functionally on the chemistry of non-covalent interactions.

CHEM291SEC02.2: Green Methods in Chemistry

(Credits: 05, 60 Lectures, Full Marks: 50)

Course Objectives: To impart knowledge on environmentally benign green methods in chemistry.

Theory and Hand-on Experiments

Introduction, Definitions of Green Chemistry, Brief introduction of twelve principles of Green Chemistry with examples, Special emphasis on atom economy, toxicity reduction, and green solvents, Green Chemistry and catalysis, and alternative sources of energy, green energy, and sustainability.

Surfactants for carbon dioxide – Replacing smog producing and ozone depleting solvents with CO_2 for precise cleaning and dry cleaning of garments, Designing of environmentally safe marine antifoulant, Right fit pigment: Synthetic azo pigments to replace toxic organic and inorganic pigments. An efficient, green synthesis of a compostable and widely applicable plastic (poly lactic acid) made from corn.

Practical

1. Preparation and characterization of biodiesel from vegetable oil.
2. Extraction of D-limonene from orange peel using liquid CO_2 prepared from dry ice.
3. Mechano chemical solvent free synthesis of azomethine.
4. Solvent free, microwave assisted one pot synthesis of phthalocyanine complex of Cu(II).

Reference Books:

- Anastas, P. T. & Warner, J. K. *Green Chemistry-Theory and Practical*, Oxford University Press (1998).
- Matlack, A. S. *Introduction to Green Chemistry*, Marcel Dekker (2001).
- Cann, M. C. & Connely, M. E. *Real-World cases in Green Chemistry*, American Chemical Society, Washington (2000).
- Ryan, M. A. & Tinnesand, M. *Introduction to Green Chemistry*, American Chemical Society, Washington (2002).
- Sharma, R. K.; Sidhwani, I. T. & Chaudhari, M. K. *Green Chemistry Experiments: A monograph,* I. K. International Publishing House (2012).
- Lancaster, M. *Green Chemistry: An introductory text*, 2nd Ed., RSC publishing (2010).
- Sidhwani, I. T.; Saini, G.; Chowdhury, S.; Garg, D.; Malovika, G.; *Wealth from waste: A green method to produce biodiesel from waste cooking oil and generation of*

useful products from waste further generated "A Social Awareness Project"., Delhi University Journal of Undergraduate Research and Innovation, 1(1), 2015.

Course Learning Outcomes: After completion of this course students should be able to

1. Design and develop green synthetic protocol using alternative greener energy sources to minimize the environmental impact of chemical reactions for sustainable development.
2. Get hands on experience of extraction and characterization of natural products and their synthesis.

CHEM292VAC02: INDUSTRIAL CHEMISTRY

(Credits: Theory-03, 30 Lectures, Full Marks: 50)

Course Objectives: The course aims to provide the knowledge on industrially important compounds and their use in everyday life. Also, may explore the industrial visit to understand the bulk production of such materials.

Fertilizers: Introduction, classification of fertilizer, manufacturing process and uses: Urea, Ammonium nitrate, Calcium ammonium nitrate, Ammonium phosphates; Polyphosphate, Super phosphate, Compound and mixed fertilizers Potassium Chloride, Potassium sulphate. **(6 Lectures)**

Chemistry of Inorganic Cementing Materials: Introduction to lime, gypsum plaster & cement, History of cementing materials, Classification of cement, Raw materials for Portland cement, Manufacturing processes of cement, Influences of minor constituents, Chemical analysis & Quality control of Portland cement, Special cement, Hydration of cement **(6 Lectures)**

Batteries and Energy Storage: Applications of batteries in daily life, Classification of batteries: Non-rechargeable & Rechargeable, Different types of rechargeable batteries: Lead acid batteries, Lithium ion batteries, Alkaline batteries, Energy storage performances: Capacity, Columbic efficiency, Energy density, power density, Cycle life, Manufacturing, Recycling, Environmental impacts, Commercial viability **(6 Lectures)**

Industrial Wastewater Treatment: Impacts of industrial wastewater in environment, Industry specific contaminants, Detection of contaminants: Chemical sensing, Treatment methods, Indian and global scenario **(6 Lectures)**

Forensic Chemistry: Introduction, Definition, Scope & Significance. Types of cases/exhibits, preliminary screening, presumptive test (color and spot test), microchemical methods of analysis, examination procedures involving standard methods and instrumental techniques, analysis of trace evidences, dyes. **(6 Lectures)**

Excursion: Visit to industries/R&D Labs, Submission of excursion report

Reference Book:

B. K. Sharma, Industrial Chemistry. Goel Publications, 1991.

K. H. Buchel, Industrial Inorganic Chemistry, Wiley-VCH, 2000

Ullmann's Encyclopedia of Industrial Chemistry, Wiley-VCH, 2011

Course Learning Outcomes: On completion of the course, the students will be familiar with chemistry of- several commercial products and forensic science.

CHEM 255MC04

Theory: TRANSITION METAL & COORDINATION CHEMISTRY, STATES OF MATTER & CHEMICAL KINETICS

(Credits: 04, 60 Lectures, Full Marks: 70)

Course Objectives: The course aims to provide the knowledge on introduction to coordination compounds, comparison of inherent properties of transition metals in group to general science students. Handful experience on qualitative analysis of inorganic salts.

Section A: Inorganic Chemistry

Coordination Chemistry

Valence Bond Theory (VBT): Inner and outer orbital complexes of Cr, Fe, Co, Ni and Cu (coordination numbers 4 and 6). Structural and stereoisomerism in complexes with coordination numbers 4 and 6. Drawbacks of VBT. IUPAC system of nomenclature. **(12 Lectures)**

Crystal Field Theory

Crystal field effect, octahedral symmetry. Crystal field stabilization energy (CFSE), Crystal field effects for weak and strong fields. Application and limitations of CFSE, Tetrahedral symmetry. Factors affecting the magnitude of Dq. Spectrochemical series. Comparison of CFSE for O_h and T_d complexes, Tetragonal distortion of octahedral geometry.

Jahn-Teller distortion, Square planar coordination. MOT elementary idea **(18 Lectures)**

Section B: Physical Chemistry

Course Objectives: To impart knowledge on the different states of matter and kinetics of chemical reactions

Kinetic Theory of Gases

Postulates of Kinetic Theory of Gases and derivation of the kinetic gas equation.

Deviation of real gases from ideal behaviour, compressibility factor, causes of deviation. Van der Waals equation of state for real gases. Boyle temperature (derivation not required). Critical phenomena, critical constants and their calculation from van der Waals equation. Andrews isotherms of CO_2.

Maxwell Boltzmann distribution laws of molecular velocities and molecular energies (graphic representation – derivation not required) and their importance.

Temperature dependence of these distributions. Most probable, average and root mean square velocities (no derivation). Collision cross section, collision number, collision frequency, collision diameter and mean free path of molecules. Viscosity of gases and effect of temperature and pressure on coefficient of viscosity (qualitative treatment only). **(8 Lectures)**

Liquids

Surface tension and its determination using stalagmometer. Viscosity of a liquid and determination of coefficient of viscosity using Ostwald viscometer. Effect of temperature on surface tension and coefficient of viscosity of a liquid (qualitative treatment only). **(6 Lectures)**

Solids

Forms of solids. Symmetry elements, unit cells, crystal systems, Bravais lattice types and identification of lattice planes. Laws of Crystallography - Law of constancy of interfacial angles, Law of rational indices. Miller indices. X–Ray diffraction by crystals, Bragg's law. Structures of NaCl, KCl and CsCl (qualitative treatment only). Defects in crystals. Glasses and liquid crystals. **(8 Lectures)**

Chemical Kinetics

The concept of reaction rates. Effect of temperature, pressure, catalyst and other factors on reaction rates. Order and molecularity of a reaction. Derivation of integrated rate equations for zero, first and second order reactions (both for equal and unequal concentrations of reactants). Half–life of a reaction. General methods for determination of order of a reaction. Concept of activation energy and its calculation from Arrhenius equation.

Theories of Reaction Rates: Collision theory and Activated Complex theory of bimolecular reactions. Comparison of the two theories (qualitative treatment only). **(8 Lectures)**

Reference Books:

- Barrow, G.M. *Physical Chemistry* Tata McGraw-Hill (2007).
- Lee, J.D. Concise Inorganic Chemistry ELBS, 1991.
- R. P. Sarkar, General and Inorganic Chemistry (Vol. 2), New Central Book Agency, ed. 3, 2011
- Huheey, J. E.; Keiter, E.A. & Keiter, R.L. Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed., Harper Collins 1993, Pearson,2006.
- Castellan, G.W. *Physical Chemistry* 4th Ed. Narosa (2004).
- Kotz, J.C., Treichel, P.M. & Townsend, J.R. *General Chemistry* Cengage Learning India Pvt. Ltd., New Delhi (2009).
- Mahan, B.H. *University Chemistry* 3rd Ed. Narosa (1998).
- Petrucci, R.H. *General Chemistry* 5th Ed. Macmillan Publishing Co.: New York (1985).
- Cotton, F.A. & Wilkinson, G. *Basic Inorganic Chemistry,* Wiley.
- Shriver, D.F. & Atkins, P.W. *Inorganic Chemistry*, Oxford University Press.
- Wulfsberg, G. *Inorganic Chemistry,* Viva Books Pvt. Ltd.
- Rodgers, G.E. *Inorganic &Solid State Chemistry,* Cengage Learning India Ltd., 2008.

CHEM255MC04-Lab: (Credits: 02, 60 Lectures, Full Marks: 30)

Section A: Inorganic Chemistry

Semi-micro qualitative analysis (using H_2S or other methods) of mixtures - two ionic species out of the following:

Cations : NH_4^+, Pb^{2+}, Cu^{2+}, Fe^{3+}, Co^{2+}, Ni^{2+}, Mn^{2+}, Ba^{2+}, K^+

Anions : S^{2-}, NO_2^-, Cl^-, Br^-, I^-, NO_3^-, SO_4^{2-}, BO_3^{3-}

Section B: Physical Chemistry

(I) Surface tension measurement (use of organic solvents excluded).

a) Determination of the surface tension of a liquid or a dilute solution using a stalagmometer.

b) Study of the variation of surface tension of a detergent solution with concentration.

(II) Viscosity measurement (use of organic solvents excluded).

a) Determination of the relative and absolute viscosity of a liquid or dilute solution using an Ostwald's viscometer.

b) Study of the variation of viscosity of an aqueous solution with concentration of solute.

(III) Chemical Kinetics

Study the kinetics of the following reactions.

Integrated rate method:

a. Acid hydrolysis of methyl acetate with hydrochloric acid.

b. Saponification of ethyl acetate.

c. Compare the strengths of HCl and H_2SO_4 by studying kinetics of hydrolysis of ester.

Reference Books:

- Svehla, G. *Vogel's Qualitative Inorganic Analysis*, Pearson Education, 2012.
- Mendham, J. *Vogel's Quantitative Chemical Analysis*, Pearson, 2009.
- Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry,* R. Chand & Co.: New Delhi (2011).

Course Learning Outcomes: On completion of the course, the students should be able to

1. Differentiate double-salts and coordination complexes.
2. Explain the structure, spectral and magnetic properties of coordination complexes
3. Predict spectral properties using various theory of coordination chemistry
4. Explain the kinetic molecular model of gas, viscosity of gas and liquids.
5. Manipulate the gas laws to describe real and ideal gas behaviour.
6. Derive rate laws of various elementary and complex reactions

SEMESTER- V

CHEM341SI01: Summer Internship

(Credits: Theory-04, Full Marks: 50)

Course Objectives: To impart experiential learning through summer Intership

The student will join summer internship programme in various research institutes/universities to have a hands-on experience on the research work carried out in a different research laboratory

Course Learning Outcomes: After the completion of the course, the students should be able to

1. Explore new areas of research in both chemistry and allied fields of science and technology.

CHEM301C09: INORGANIC CHEMISTRY-IV

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Course Objectives: The course aims to provide the knowledge on introductory level organometallic chemistry, Introduce the enzymes, concept of drugs and toxicity of heavy metals in life. Introduce the various electroanalytical techniques and various aspects of environmental chemistry. Also introduce the hands-on training on qualitative inorganic salt analysis.

Basics of Organometallic Chemistry:

Definition and classification of organometallic compounds on the basis of bond type. Concept of hapticity of organic ligands. Metal carbonyls: 18-electron and 16-electron rule and its application, electron count of mononuclear, polynuclear and substituted metal carbonyls of 3d series. General methods of preparation (direct combination, reductive carbonylation, thermal and photochemical decomposition) of mono and binuclear carbonyls of 3d series. Structures of mononuclear and binuclear carbonyls of Cr, Mn, Fe, Co and Ni using VBT. π-acceptor behaviour of CO (MO diagram of CO to be discussed), synergic effect and use of IR data to explain extent of back bonding. Zeise's salt: Preparation and structure, evidences of synergic effect and comparison of synergic effect with that in carbonyls.

Ferrocene: Preparation and reactions (acetylation, alkylation, metallation, Mannich Condensation). Structure and aromaticity. Comparison of aromaticity and reactivity with that of benzene.

Metal Alkyls: Important structural features of methyl lithium (tetramer) and trialkyl aluminium (dimer), concept of multicentre bonding in these compounds. Role of triethylaluminium in polymerisation of ethene (Ziegler – Natta Catalyst). Species present in ether solution of Grignard reagent and their structures, Schlenk equilibrium. **(28 Lectures)**

Bioinorganic Chemistry-2:

Carboxypeptidase, carbonic anhydrase. biological nitrogen fixation, Photosynthesis: Photo system-I and Photosystem-II. Toxic metal ions and their effects, chelation therapy, Pt and Au complexes as drugs, metal dependent diseases. superoxide dismutase (SOD), cytochrome C oxidase; respiratory electron transport chain, metal dependent diseases. **(8 Lectures)**

Electroanalytical Chemistry

Electrochemical cells; Types of electrodes; Reference electrodes; Polarization effects: Concentration and Kinetic polarizations; Linear scan voltammetry: Hydrodynamic voltammetry and Polarography;

Cyclic voltammetry; Electrogravimetry; Coulometry; Electrochemical impedance spectroscopy

(16 Lectures)

Environmental Chemistry

Air pollution and its effects, air quality standards, photochemical smog, major primary pollutants produced by human activity: sulphur oxides (SOx), nitrogen oxides (NOx), carbon monoxide, carbon dioxide, volatile organic compounds, particulate matter, persistent free radicals, toxic metals, chlorofluorocarbons, aerosols

Ozone chemistry, ozone layer and its depletion, global warming and greenhouse effect, greenhouse gases, carbon footprint, the Albedo effect, acid rain and its effect, measurement of acid rain, ocean acidification and its biological impact

water pollution, major types of water pollution and its causes, chemical waste, biochemical oxygen demand (BOD), chemical oxygen demand (COD), total dissolved solids (TDS), total suspended solid (TSS) in water samples, water treatment, coagulation and flocculation, chemical treatment and disinfection process of drinking water, ion exchange process for water treatment, advanced oxidation process, photochemical process **(8 lectures)**

Reference Books:

- Huheey, J. E.; Keiter, E.A. & Keiter, R.L. Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed., Harper Collins 1993, Pearson,2006.
- A. Elias, B. D. Gupta, Basic Organometallic Chemistry, Universities Press (ed. 2), 2013.
- Powell, P. Principles of Organometallic Chemistry, Chapman and Hall, 1988.
- Shriver, D.D. & P. Atkins, Inorganic Chemistry 4nd Ed., Oxford University Press, 1994.
- Miessler, G. L. & Tarr, D.A. Inorganic Chemistry 4th Ed., Pearson, 2010.
- Crabtree, R. H. The Organometallic Chemistry of the Transition Metals. New York, NY: John Wiley, 2000.
- Spessard, G. O. & Miessler, G.L. Organometallic Chemistry. Upper Saddle River, NJ: Printice-Hall, 1996.
- Asim K Das, Bioinorganic Chemistry
- Willard, H.H. *et al.*: *Instrumental Methods of Analysis*, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
- Christian, G.D. *Analytical Chemistry*, 6th Ed. John Wiley & Sons, New York, 2004.
- Harris, D.C.: *Exploring Chemical Analysis*, 9th Ed. New York, W.H. Freeman, 2016.
- Khopkar, S.M. *Basic Concepts of Analytical Chemistry*. New Age International Publisher, 2009.
- Skoog, D.A. Holler F.J. & Nieman, T.A. *Principles of Instrumental Analysis*, Cengage Learning India Ed.
- Anil. K. De, Environmental Chemistry, New Age Publishers Pvt Ltd, 9th Ed. 2018

Inorganic Qualitative Analysis - 2 CHEM301C09 LAB

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

Cation radicals derived from:

Na, K, NH_3, Mg, Ca, Sr, Ba, Al, Pb, Cr, Mn, Fe, Co, Ni, Cu, Zn

Anion radicals:

F^-, CI^-, Br^-, I^-, NO_3^-, NO_2^-, SCN^-, S^{2-}, SO_4^{2-}, $S_2O_3^{2-}$, PO_4^{3-}, BO_3^{3-}, CrO_4^{2-}

Detection of four radicals by macro, semi- micro tests. Mixtures should preferably contain one interfering anion, or insoluble component ($BaSO_4$, $SrSO_4$, $PbSO_4$, CaF_2 or Al_2O_3) or combination of anions Spot tests should be done whenever possible.

Reference Books

- Vogel's Qualitative Inorganic Analysis, Revised by G. Svehla. Pearson Education, 2002.
- G. N. Mukherjee, Hand Book of Inorganic Analysis, U. N. Dhar & sons (P) LTD, 2014
- Marr & Rockett Practical Inorganic Chemistry. John Wiley & Sons 1972.

Course Learning Outcomes: On completion of the course, the students should be able to

1. Know the theoretical and practical knowledge on separation and analysis of individual inorganic cations and anions.
2. Find the composition of unknown inorganic salt combinations.
3. Perform electron count and calculate stability of organometallic compounds
4. Able to explain the structural features of organometallic compounds
5. Explain the concept of drug and their interaction with enzymes in our body
6. Describe the metal-based drugs and their side effects.
7. Demonstrate the metal inducing pollution to environment; living system and some possible remedy.
8. Able to explain the concept of different electroanalytical cells
9. Interpret data from modern electrochemical method such as voltammetry and Coulometry
10. Able to explain the sources of different pollutions and their detrimental effect of environment

CHEM302C10: ORGANIC CHEMISTRY-III

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Course Objectives: To impart knowledge on the chemistry of nitrogenous compounds, polynuclear hydrocarbons, heterocycles, and synthetic strategies of organic compounds.

Nitrogen Containing Functional Groups

Preparation and important reactions of nitro, nitriles and isonitrile compounds. Effect of substituents and solvent on the basicity of amines, Gabriel phthalimide synthesis, Carbylamine reaction, Mannich reaction, Hoffmann's exhaustive methylation, Hofmann-elimination reaction. Distinction between 1°, 2° and 3°-amines with Hinsberg reagent and nitrous acid. Preparation and synthetic applications of Diazonium salts. **(20 Lectures)**

Polynuclear Hydrocarbons

Reactions of naphthalene, phenanthrene and anthracene. Structure elucidation, preparation, and important derivatives of naphthalene and anthracene, Polynuclear hydrocarbons.

Synthetic Strategy

Retrosynthetic analysis – disconnections, synthons, donor and acceptor synthons, functional group interconversion, C-C disconnections and synthesis [one group and two group (1,2 to 1,6-deoxygenated), reconnection (1,6-dicarbonyl), natural reactivity and umpolung, protection-deprotection strategy (alcohol, amine, carbonyl, acid).

(20 Lectures)

Heterocyclic Compounds

Classification, nomenclature, structure, aromaticity in 5- and 6-membered rings bearing one heteroatom. Synthesis, reactions and mechanism of substitution reactions of Furan, Pyrrole (Paal-Knorr synthesis, Knorr pyrrole synthesis, Hantzsch synthesis), Thiophene, Pyridine (Hantzsch synthesis), Pyrimidine. Structure elucidation of indole, Fischer indole and Madelung synthesis. Structure elucidation of quinoline and isoquinoline, Skraup synthesis, Friedlander synthesis, Knorr quinoline synthesis, Doebner-Miller synthesis, Bischler-Napieralski reaction, Pictet-Spengler reaction, Pomeranz-Fritsch reaction. Derivatives of furan: Furfural and furoic acid. **(20 Lectures)**

Reference Books:

- Finar, I. L. *Organic Chemistry (Vol. I)*, 6th Ed., Pearson (2002).
- Finar, I. L. *Organic Chemistry* (*Vol. II)*, Pearson (2002).
- Acheson, R. M. *Introduction to the Chemistry of Heterocyclic compounds*, John Welly & Sons (1976).
- Graham Solomons, T. W.; Fryhle, C. B. & Snyder, S. A. *Organic Chemistry,* 12th Ed., John Wiley & Sons (2017).
- Clayden, J.; Greeves, N. & Warren, S. *Organic Chemistry*, 2nd Ed., Oxford University Press (2012).
- Warren S. *Organic Synthesis: The disconnection Approach*, Wiley (2008).

CHEMISTRY PRACTICAL- CHEM302C10 LAB

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

1. Chromatography and determination of R_f values.

(a) Separation of a mixture of two amino acids by ascending and horizontal paper chromatography.

(b) Separation of a mixture of two sugars by ascending paper chromatography.

(c) Separation of a mixture of *o*- and *p*-nitrophenol or *o*- and *p*-aminophenol by thin layer chromatography (TLC).

2. Extraction and purification of natural products and biomolecules.

3. Analysis of carbohydrates: aldoses and ketoses, reducing and non-reducing sugars.

4. Estimation of glycine by Sorenson's formalin method.

5. Study of the titration curve of glycine.

6. Estimation of Vitamin C.

Reference Books:

- Mann, F. G. & Saunders, B. C. *Practical Organic Chemistry*, Pearson (2009).
- Furniss, B. S.; Hannaford, A. J.; Smith, P. W. G. & Tatchell, A. R. *Vogel's Textbook of Practical Organic Chemistry*, 5th Ed., Pearson (2012).
- Ahluwalia, V. K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis*, University Press (2000).
- Ahluwalia, V. K. & Dhingra, S. *Comprehensive Practical Organic Chemistry: Qualitative Analysis*, University Press (2000).

Course Learning Outcomes: After completion of the course, the student should be able to

1. Explain physical and chemical properties of nitrogen bearing organic molecules (amines, diazonium salts, nitro, nitriles, and isonitriles) and their effects on reactivity together with their preparations and synthetic applications.
2. Elucidate structures, a variety of preparative methods and reactions of polynuclear hydrocarbons.
3. Explicate structures, and synthesis of several heterocycles: Furan, Pyrrole, Thiophene, Pyridine, Pyrimidine, Indole, Quinoline, and Isoquinoline.
4. Plan retrosynthetic strategies to develop basic organic transformations.
5. Analyse unknown organic compounds, carbohydrates, amino acids in a qualitative manner, perform chromatographic separations and solvent extraction which will augment their analytical skill.

CHEM303C11: PHYSICAL CHEMISTRY-IV

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Course Objectives: To acquire knowledge of the quantum chemical description of various chemical systems, conductance and electrical and magnetic properties of atoms and molecules and solid state chemistry.

Quantum Chemistry-I

Breakdown of classical ideas – Line Spectra, black body (or cavity) radiation, Planck's quantization, photoelectric effect, Elementary idea of Bohr Theory, Compton scattering for relativistic (preliminary idea only); wave properties of particles: de Broglie hypothesis and the concept of matter waves, Davisson-Germer experiment, nature of matter waves: group and phase velocities and the idea of a wave packet; Heisenberg uncertainty principle and its relation to the measurement process, Differentiation of small and large particles on the basis of Uncertainty Principle, necessity of more general theory.

Time-independent form of the Schrödinger equation; probabilistic interpretation of the wave function; conditions for acceptability of wave functions.

Postulates of quantum mechanics, quantum mechanical operators, Schrödinger equation and its application to free particle and "particle-in-a-box" (rigorous treatment), quantization of energy, zero-point energy and Heisenberg Uncertainty principle; wavefunctions, probability distribution functions, nodal properties, Extension to two- and three-dimensional boxes, separation of variables, degeneracy; Barrier potential, Tunnelling.

(20 Lectures)

Conductance

General Law for charge transfer, Comparison of conduction in solutions and metals, Arrhenius theory of electrolytic dissociation. Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Molar conductivity at infinite dilution. Kohlrausch law of independent migration of ions. Structure of ionic solutions, Debye-Hückel law (with derivation), Debye-Hückel-Onsager equation, Wien effect, Debye-Falkenhagen effect, Walden's rules, Temperature and viscosity dependence of conductivity, abnormal conductivity of H^+ and OH^- ions, Grotthuss mechanism, Ionic velocities, mobilities and their determinations, transference numbers and their relation to ionic mobilities, determination of transference numbers using Hittorf and Moving Boundary methods. Applications of conductance measurement: (i) degree of dissociation of weak electrolytes, (ii) ionic product of

water (iii) solubility and solubility product of sparingly soluble salts, (iv) conductometric titrations, and (v) hydrolysis constants of salts. **(20 Lectures)**

Solid state

Nature of the solid state, law of constancy of interfacial angles, law of rational indices, Miller indices, elementary ideas of symmetry, symmetry elements and symmetry operations, qualitative idea of point and space groups, seven crystal systems and fourteen Bravais lattices; X-ray diffraction, Bragg's law, a simple account of rotating crystal method and powder pattern method. Analysis of powder diffraction patterns of NaCl, CsCl and KCl. Defects in crystals. Glasses and liquid crystals. **(10 Lectures)**

Electrical & Magnetic Properties of Atoms and Molecules

Basic ideas of electrostatics, electric field, Gauss law, concept of electric potential, Poisson's equation, electric field due to point dipole, energy of a dipole in an electric field, polarizability (distortion and orientational), Electrostatics of dielectric media, relation between polarization and surface charge density, Clausius-Mosotti equation, estimation of orientational polarizability, Debye equation, Lorenz-Laurentz equation, Measurements of Dipole moment and molecular polarizabilities.

Spin and orbital contribution in magnetic moment, Diamagnetism, paramagnetism, ferromagnetism and anti-ferromagnetism; magnetic susceptibility and its measurement (Gouy's method, SQUID), Temperature dependence of magnetic susceptibility, Curie's equation.

(10 Lectures)

Reference Books:

- Levine. I. N., Quantum Chemistry 7th Ed. Pearson (2016)
- McQuarrie. D. A., Quantum Chemistry Viva Student Ed. Pearson (2003)
- Atkins, P.W & Paula, J.D. Physical Chemistry, 10th Ed., Oxford University Press(2014).
- Castellan, G. W. Physical Chemistry 4th Ed., Narosa (2004).
- Mortimer, R. G. Physical Chemistry 3rd Ed., Elsevier: NOIDA, UP (2009).
- Barrow, G. M., Physical Chemistry 5th Ed., Tata McGraw Hill: New Delhi (2006).
- Engel, T. & Reid, P. Physical Chemistry 3rd Ed., Prentice-Hall (2012).
- Rogers, D. W. Concise Physical Chemistry Wiley (2010)
- Silbey, R. J.; Alberty, R. A. &Bawendi, M. G. Physical Chemistry 4th Ed., JohnWiley & Sons, Inc. (2005).
- Wolfson, M. M., An Introduction to X-Ray Crystallography, 2nd Ed., Cambridge University Press (1997).

CHEMISTRY PRACTICAL- CHEM303C11 LAB

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

1. pH metry

(i) Study the effect on pH of addition of HCl/NaOH to solutions of acetic acid, sodium acetate and their mixtures.

(ii) Preparation of buffer solutions of different pH

(a) Sodium acetate-acetic acid

(b) Ammonium chloride-ammonium hydroxide

(iii) pH metric titration of

(a) strong acid vs. strong base

(b) weak acid vs. strong base.

(iv) Determination of dissociation constant of a weak acid.

2. Conductometry

(i) Determination of cell constant

(ii) Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid.

(iii) Perform the following conductometric titrations:

(a) Strong acid vs. strong base

(b) Weak acid vs. strong base

(c) Mixture of strong acid and weak acid vs. strong base

(d) Strong acid vs. weak base

(iv) Determination of CMC of surfactants using conductometry

3. Indexing of a given powder diffraction pattern of a cubic crystalline system.

Reference Books:

- Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011).
- Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry
  8th Ed.; McGraw-Hill: New York (2003).
- Halpern, A. M. & McBane, G. C. Experimental Physical Chemistry 3rd Ed.; W.H. Freeman & Co.: New York (2003).

Course Learning Outcomes: After the completion of the course, the students should be able to

1. Recognise the importance of the quantum chemistry and quantization of energy.

2. Solve the Schrodinger equation of various particle in a box problem and apply them to real systems related to chemistry.
3. Apply the principles of electrochemistry to conductance, voltaic, and electrolytic systems.
4. Provide a physical basis for Debye-Hückel theory.
5. Analyse the powder X-ray diffraction data of cubic systems
6. Perform acid-base titration using conductometric method.
7. Explain the concepts of electrical and magnetic properties of atoms and molecules.

SEMESTER- VI

CHEM351C12: INORGANIC CHEMISTRY-V

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Course Objectives: The course aims to provide the knowledge on different types of organometallic reactions, mechanistic pathway of organic transformations using organometallic reagents. To provide an introduction into symmetry of molecules. Also provide the knowledge on some physical aspects of coordination complexes.

Advanced Organometallic Chemistry

Reaction of organometallic complexes: substitution, oxidative addition, reductive elimination, insertion and elimination, electrophilic and nucleophilic reactions of coordinated ligands. Stereochemical non-rigidity and fluxional behaviour of organometallic compounds with typical examples.

Catalysis by organometallic compounds: Hydrogenation of unsaturated compounds, Wilkinson's catalyst, Tolman catalytic loop; Syntheses gas- water gas Shift reaction; Hydroformylation (oxo process); Monsanto acetic acid process; Wacker process, synthetic gasoline-Fischer-Tropsch process; polymerization, oligomerization and metatheses reaction of alkenes and alkynes, C-N bond coupling reactions. **(20 Lectures)**

Principles of Symmetry in Chemistry

Concept of symmetry in molecules, symmetry elements and symmetry operations, products of symmetry operations, multiplication table by stereographic projection technique. Elements of group theory, Sub groups and classes of group elements, Symmetry point groups of molecules, systematic classification of molecular point groups.

Unit vector transformation, matrix representation of symmetry, matrix diagonalizations, reducible and irreducible representations, construction of character table, Mulliken symbols for irreducible representations, interpretation of character table, transformation properties of atomic orbitals and basis functions

Application of group theory in identifying polar and chiral molecules. Symmetry and stereo-isomerism. Utilization of symmetry and projection operation to construct SALC of ligand group orbitals. Constructing of qualitative MO energy diagram of polyatomic molecules (H_2O, BeH_2, NH_3, BH_3).

MO diagrams of coordination complexes (sigma bonding & pi-bonding). Selection rules in molecular spectroscopy, Application of group theory to find symmetry of normal modes, selection rules for IR and Raman transitions. **(25 lectures)**

Advanced Coordination chemistry:

Thermodynamic aspects of crystal field splitting, kinetics aspects of crystal field splitting, Mulliken Term symbols and its applications, Correlation of LFT with charge transfer spectra, spectral calculations, Structural aspects and stereoisomerism of coordination compounds, enumeration of isomers, optically active coordination compounds and their resolution procedures, absolute configuration of enantiomers. **(15 Lectures)**

Reference Books:

- Huheey, J. E.; Keiter, E.A. & Keiter, R.L. Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed., Harper Collins 1993, Pearson,2006.
- A. Elias, B. D. Gupta, Basic Organometallic Chemistry, Universities Press (ed. 2), 2013.
- Powell, P. Principles of Organometallic Chemistry, Chapman and Hall, 1988.
- Shriver, D.D. & P. Atkins, Inorganic Chemistry 4nd Ed., Oxford University Press, 1994.
- Miessler, G. L. & Tarr, D.A. Inorganic Chemistry 4th Ed., Pearson, 2010.
- Crabtree, R. H. The Organometallic Chemistry of the Transition Metals. New York, NY: John Wiley, 2000.
- Spessard, G. O. & Miessler, G.L. Organometallic Chemistry. Upper Saddle River, NJ: Printice-Hall, 1996.
- F.Albert Cotton, Chemical Applications of Group Theory, Wiley India, 2003.
- S. K. Dogra, H. S. Randhawa, Symmetry and Group Theory in Chemistry, New Academic Science, 2017
- Symmetry and Spectroscopy of Molecules - K. V. Reddy.
- Group Theory in Chemistry - A. K. Mukherjee, B. C. Ghosh.
- Purcell, K.F & Kotz, J.C. Inorganic Chemistry W.B. Saunders Co, 1977.

Inorganic Advanced Synthesis CHEM351C12 Lab

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

(A) Synthesis and characterization of Inorganic Compounds

Preparation of transition metal complexes and their characterization

(B) **Colorimetric Analysis**

1. Determination of composition of complexes by continuous variation / Mole ratio / Slope ratio method of the following systems: Fe (III) – sulphosalicylate complex; Fe (II) - phenanthroline complex

2. Colorimetric study of the kinetics of inorganic reaction

Reference Books

- G. N. Mukherjee, Hand Book of Inorganic chemistry, U. N. Dhar & sons (P) LTD, 2014
- Marr & Rockett Practical Inorganic Chemistry. John Wiley & Sons 1972.

Course Learning Outcomes: On completion of the course, the students should be able to

1. Able to explain the fundamental reaction types of organometallic compounds and the mechanisms in the organometallic catalytic processes.
2. Able to explain the industrial and commercial importance of organometallic catalysis
3. Recognize symmetry elements in a molecule and deduce point group. Can represent matrices for symmetry representation.
4. Use character table to find out the symmetry labels for any orbitals and basis functions, which is extensively used in spectroscopy course. They will also be able to construct qualitative MOED diagram using character table.
5. Able to explain the various physiochemical aspects of coordination complexes using different theories of coordination complexes
6. Able to execute the new synthesis on their own

CHEM352C13: ORGANIC CHEMISTRY-IV

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Course Objectives: To impart knowledge on organic spectroscopic techniques, organometallic chemistry, and pericyclic reactions.

Organic Spectroscopy

UV Spectroscopy: Types of electronic transitions, λ_{max}, Chromophores and auxochromes, Bathochromic and hypsochromic shifts, Intensity of absorption, Application of Woodward rules to calculate λ_{max} for the following systems: α,β-unsaturated aldehydes, ketones, carboxylic acids, esters, conjugated dienes (alicyclic, homoannular and heteroannular), extended conjugated systems (aldehydes, ketones and dienes), and distinction between *cis*- and *trans*-isomers.

IR Spectroscopy: Fundamental and non-fundamental molecular vibrations, IR absorption positions of O, N and S containing functional groups, Effect of H-bonding, conjugation, resonance and ring size on IR absorptions, Fingerprint region and its significance, and application in functional group analysis.

NMR Spectroscopy: Basic principles of Proton Magnetic Resonance, chemical shift, shielding and deshielding mechanisms, Anisotropic effects in alkene, alkyne, aldehydes and aromatics, equivalence and non-equivalence of protons, Spin–Spin coupling, notation for spin systems, coupling constant, and its variation with stereochemistry, Karplus equation. Structural application of ^{1}H NMR, aromaticity, antiaromaticity and homoaromaticity of organic molecules and related problems. Applications of IR, UV and NMR for identification of simple organic molecules. **(30 Lectures)**

Advanced M.O.

HMOT for acyclic conjugated π systems with even and odd number of p orbitals, carbonyl π-system, Substitution effect on Frontier orbital energies of π systems, Fulvene systems, cyclic conjugated π systems, Möbius system. **(8 Lectures)**

Pericyclic Reactions

Molecular orbitals for acyclic conjugated systems. Theory of pericyclic reactions – (i) Frontier Molecular Orbital (FMO) approach, (ii) Concept of aromaticity of transition states

(Hückel/Möbius systems), (iii) Woodward-Hoffmann selection rules and general rules. Symmetry principles in pericyclic reactions, orbital and state correlation diagram for electrocyclic and cycloaddition reactions. Reactivity, regioselectivity and periselectivity.

Electrocyclic reactions: Scope, reactivity and stereochemical features of electrocyclic reactions (4e, 6e and 8e neutral systems). Electrocyclic reactions of charged systems (cations and anions), Conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems.

Sigmatropic rearrangements: [1, j]-shifts – [1,3], [1,5] and [1,7] shifts in neutral systems and [1,4] shift in charged species: [i, j]-shifts – [3,3] shifts, Sommelet-Hauser, Cope, aza-Cope rearrangements, Fluxional tautomerism, Claisen rearrangements, [5,5]-shifts, and [2,3]-shifts in ylids.

Cycloaddition reactions: Antarafacial and suprafacial additions, 4n and 4n+2 systems; 2,2-addition of ketenes, 1,3-dipolar cycloadditions and cheleotropic reactions. Ene reactions, group-transfer reactions and eliminations. [4+2] and [2+2] reactions, cheletropic addition of carbene. **(22 Lectures)**

Reference Books:

- Kemp, W. *Organic Spectroscopy*, Macmillan India (2019).
- Pavia, D. L. *Introduction to Spectroscopy,* 5th Ed., Cengage India Pvt. Ltd. (2015).
- Woodward, R. B. & Hoffmann R. *The Conservation of Orbital Symmetry*, 1969, 8(11), 781–932.
- Gilchrist, T. L. & Storr, R. C. *Organic Reactions and Orbital Symmetry*, 2nd Ed., Cambridge University Press (1979).
- Mandal, D. K. *Pericyclic Chemistry*, 1st Ed., Elsevier (2018).
- Fleming, I. *Pericyclic Reactions,* 2nd Ed., Oxford University Press (2015).
- Fleming, I. *Molecular Orbitals and Organic Chemical Reactions,* John Wiley and Sons, Ltd., (2010).

CHEMISTRY PRACTICAL- CHEM352C13 LAB

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

1. Identification of simple organic compounds by IR and NMR spectroscopy (Spectra to be provided)

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Reference Books:

- Kemp, W. *Organic Spectroscopy*, Macmillan India (2019).
- Pavia, D. L. *Introduction to Spectroscopy,* 5th Ed., Cengage India Pvt. Ltd. (2015).

- Dyer *Applications of Absorption Spectroscopy of Organic Compounds*, Prentice Hall India Learning Pvt. Ltd. (1978).

Course Learning Outcomes: After completion of the course, the student should be able to

1. Explain the principles and instrumentation techniques of UV, IR and NMR spectroscopy and interpret the spectra to characterize simple organic molecules which will also increase their analytical skill.
2. Understand the preliminary idea of pericyclic reactions: Electrocyclic reactions, Sigmatropic rearrangements and Cycloadditions and explain their feasibility in light of FMO and Woodward-Hoffmann rules.

CHEM353C14: PHYSICAL CHEMISTRY-V

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Course Objectives: To impart knowledge on the various quantum mechanical models, statistical concept of thermodynamics, fundamentals of rotation, vibration, Raman, spectroscopy and basic ideas of Photochemistry and Photoluminescence.

Quantum Chemistry-II

Qualitative treatment of simple harmonic oscillator model of vibrational motion: Setting up of Schrödinger equation and its solution. Symmetric and anti-symmetric Wavefunctions. Vibrational energy of diatomic molecules and zero-point energy.

Rigid rotator model of rotation of diatomic molecule. Schrödinger equation, transformation to spherical polar coordinates. Separation of variables. Spherical harmonics. Discussion of solution.

Angular momentum: Commutation rules, quantization of square of total angular momentum and z-component.

Qualitative treatment of hydrogen atom and hydrogen-like ions: setting up of Schrödinger equation in spherical polar coordinates, radial part, quantization of energy (only final energy expression). Average and most probable distances of electron from nucleus.

Setting up of Schrödinger equation for many-electron atoms (He, Li). Spin, Antisymmetry and Pauli exclusion principle.

(18 Lectures)

Statistical Thermodynamics and Third Law

Statement of third law, concept of residual entropy, calculation of absolute entropy of molecules

Concept of probability. Micro- and macrostates, thermodynamic probability, entropy and probability, the Boltzmann-Planck entropy formula, the Maxwell-Boltzmann distribution law for the distribution of molecular energies, Partition function: translational (for ideal gas - concept of thermal wavelength), rotational, vibrational and electronic partition functions (diatomic molecule); molecular and molar partition function, thermodynamic quantities from partition function, Einstein's theory of heat capacity of solids, the characteristics temperature, its limitations and Debye's modification thereof ; Nernst heat theorem, approach to zero Kelvin, adiabatic demagnetization, Planck's formulation of third law and the concept of absolute entropies.

Qualitative idea of Quantum statistics (Bose-Einstein, Fermi-Dirac statistics): Thermodynamic probability and distribution formula (without derivation), comparison with classical statistics - distinguishability and indistinguishability of identical particles.

(18 Lectures)

Molecular Spectroscopy

Unifying Principles: Electromagnetic radiation, Interaction of electromagnetic radiation with molecules and various types of spectra, Line width, Selection rules, Intensity of spectral lines, Born-Oppenheimer approximation (qualitative idea), Rotational, Vibrational and Electronic energy levels.

Rotation spectroscopy: Selection rules, intensities of spectral lines, determination of bond lengths of diatomic and linear triatomic molecules, isotopic substitution.

Vibrational spectroscopy: Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies, fundamental frequencies, overtones, hot bands, degrees of freedom for polyatomic molecules, modes of vibration, concept of group frequencies. Vibration-rotation spectroscopy: diatomic vibrating rotator, P, Q, R branches.

Raman spectroscopy: Qualitative treatment of Rotational Raman effect; Effect of nuclear spin, Vibrational Raman spectra, Stokes and anti-Stokes lines; their intensity difference, rule of mutual exclusion. **(18 Lectures)**

Photochemistry

Characteristics of electromagnetic radiation, Lambert-Beer's law and its limitations, physical significance of absorption coefficients. Laws, of photochemistry, quantum yield, actinometry, examples of low and high quantum yields, photochemical equilibrium and the differential rate of photochemical reactions, photosensitised reactions, quenching, chemiluminescence. Role of photochemical reactions in biochemical processes. Photochemical Reactions: kinetics of HI decomposition, H_2-Br_2 reaction, dimerization of anthracene, photo stationary state.

(6 Lectures)

Reference Books:

- Levine. I. N., Quantum Chemistry 7th Ed. Pearson (2016)
- Engel, T. & Reid, P. Physical Chemistry 3rd Ed. Pearson (2013).
- McQuarrie D. A., Statistical Thermodynamics, Harpar & Row (1973)

- Banwell, C. N. & McCash, E. M. Fundamentals of Molecular Spectroscopy 4th Ed. Tata McGraw-Hill: New Delhi (2006).
- Chandra, A. K. Introductory Quantum Chemistry Tata McGraw-Hill (2001).
- House, J. E. Fundamentals of Quantum Chemistry 2nd Ed. Elsevier: USA (2004).
- Kakkar, R. Atomic & Molecular Spectroscopy: Concepts & Applications, Cambridge University Press (2015).
- K K. Rohotgi Mukherjee, Fundamentals of Photochemistry
- Lowe, J. P. & Peterson, K. Quantum Chemistry, Academic Press (2005).

CHEMISTRY PRACTICAL- CHEM353C14 LAB

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

Colourimetry

1. Verify Lambert-Beer's law and determine the concentration of $CuSO_4/KMnO_4/K_2Cr_2O_7$ in a solution of unknown concentration
2. Study the kinetics of iodination of propanone in acidic medium.
3. Determine the amount of iron present in a sample using 1,10-phenathroline.
4. Determination isosbestic point and indicator constant
5. Study the kinetics of perdisulphate and iodide.

Performing the following DFT calculations using Gaussian 16/ ORCA software.

1. Energy minimization, structure optimization, calculating analytical frequency for simple compounds.
2. Transition state optimization, comparison of rate constants for SN2 reaction.
3. Calculating IR, UV, NMR, VCD spectra of small molecules.
4. MO analysis, population analysis (NBO) for π-conjugated systems.

Reference Books

- Khosla, B. D.; Garg, V. C. & Gulati, A., Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011).
- Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry 8th Ed.; McGraw-Hill: New York (2003).
- Halpern, A. M. & McBane, G. C. Experimental Physical Chemistry 3rd Ed.; W.H. Freeman & Co.: New York (2003).
- Exploring Chemistry with Gaussian.

Course Learning Outcomes: After the completion of the course, the students should be able to

1. Derive the vibrational and rotational energy levels of diatomic molecules using quantum mechanics
2. Explain atomic structure and the application of the concept of quantization of energy of different orbitals.
3. Demonstrate the relation between microscopic and macroscopic properties of matter.
4. Explain the structural properties of molecules on the basis of spectroscopic data
5. Calculate the quantum yield on the basis of the mechanism of photochemical reactions and explain the fates of electronically excited molecules by using Jablonski diagram
6. Apply DFT to explore reaction mechanism, bonding in molecule.

CHEM354C15: ORGANIC CHEMISTRY-V

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Course Objectives: To impart knowledge on nucleic acids, amino acids, peptides, proteins, carbohydrates, enzymes and realizing organic reactions considering Hammett Equation.

Nucleic Acids

Components of nucleic acids, Nucleosides and nucleotides. Structure, synthesis, and reactions of Adenine, Guanine, Cytosine, Uracil and Thymine. Structure of polynucleotides.

(8 Lectures)

Amino Acids, Peptides and Proteins

Amino acids, Peptides and their classification. α-amino acids - Synthesis, ionic properties and reactions. Zwitterions, pK_a values, isoelectric point and electrophoresis, Study of peptides, determination of their primary structures, end group analysis, methods of peptide synthesis. Synthesis of peptides using N-protecting, C-protecting and C-activating groups, Solid-phase synthesis. **(16 Lectures)**

Carbohydrates

Monosaccharides – Constitution and absolute configuration of glucose and fructose, epimers and anomers, mutarotation, determination of ring size of glucose and fructose. Haworth projections and conformational structures, Interconversions of aldoses and ketoses, Kiliani-Fischer synthesis, Ruff degradation, Osazone formation, Oxidation and Reduction. Disaccharides – Structure elucidation of maltose, lactose and sucrose. **(16 Lectures)**

Enzymes

Introduction, classification, and characteristics of enzymes. Salient features of active site of enzymes. Mechanism of enzyme action (taking trypsin as example), factors affecting enzyme action, coenzymes and cofactors and their role in biological reactions, specificity of enzyme action (including stereospecificity), enzyme inhibitors and their importance, phenomenon of inhibition (competitive, uncompetitive and non-competitive inhibition including allosteric inhibition). **(8 Lectures)**

Hammett Equation and its modifications

Physical significance of ρ & σ, Modifications of ρ-values as ρ^+ and ρ^-, Deviation from linearity in Hammett plot, model examples, Yukawa-Tsuno equation. **(12 Lectures)**

Reference Books:

- Finar, I. L. *Organic Chemistry, Vol. 2:Stereochemistry and the Chemistry Natural Products*, 5th Ed., Pearson (2002).
- Singh, J.; Ali, S. M. & Singh, J. *Natural Products Chemistry*, Pragati Prakashan (2010).
- Berg, J. M.; Tymoczko, J. L. & Stryer, L. *Biochemistry*, 6th Ed., W. H. Freeman (2006).
- Nelson, D. L. & Cox, M. M. *Lehninger Principles of Biochemistry*, 7th Ed., W.H. Freeman and Co. (2017).
- Kennelly, P. J. *Harper's Illustrated Biochemistry*, 32nd Ed., McGraw-Hill (2022).
- Johnson, C. D. *The Hammett Equation*, Cambridge University Press (1980).

CHEMISTRY PRACTICAL- CHEM354C15 LAB

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

1. Separation of binary mixtures of solid-solid/liquid-solid/liquid-liquid organic compounds and identification of individual components by chemical methods.

Reference Books:

- Mann, F. G. & Saunders, B. C. *Practical Organic Chemistry*, Pearson (2009).
- Furniss, B. S.; Hannaford, A. J.; Smith, P. W. G. & Tatchell, A. R. *Vogel's Textbook of Practical Organic Chemistry*, 5th Ed., Pearson (2012).
- Ahluwalia, V. K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis*, University Press (2000).
- Ahluwalia, V. K. & Dhingra, S. *Comprehensive Practical Organic Chemistry: Qualitative Analysis*, University Press (2000).

Course Learning Outcomes: After completion of the course, the students should be able to

1. Explore the fundamentals of nucleic acids, nucleosides, and nucleotides.
2. Elucidate Primary, Secondary, Tertiary and Quaternary Structure of proteins, and structure of peptides and carry out synthesis and reactions of amino acids.
3. Explain physical, chemical, and optical properties of basic units of carbohydrates.
4. Elucidate structure function relationship of enzymes in biosystems.
5. Determine a linear free-energy relationship relating reaction rates and equilibrium constants for many organic reactions.

6. Ascertain the chemical composition from a binary mixture of organic compounds.

SEMESTER- VII

CHEM401C16: Advanced Spectroscopy

(Credits: Theory-04, 60 Lectures, Full Marks: 50)

Course Objectives: To impart knowledge on the theory and application of electronic, NMR, EPR, Mössbauer, and photoelectron Spectroscopy.

Electronic Spectroscopy

Light Matter Interaction, Absorption-Emission Kinetics, Principles of LASER and characteristic features. Basic idea of spectral intensities: Fermi Golden rule and selection rules from quantum mechanical viewpoints. Relaxation of selection rules. Radiative and non-radiative deactivation of excited molecules: Fluorescence - mirror-image symmetry, Phosphorescence, radiative life time, radiation less deactivation – internal conversion and intersystem crossing, delayed fluorescence. Quenching of fluorescence, Stern-Volmer equation and plot, static and dynamic quenching, Life-time variation in presence of quencher. Fluorescence quenching study of tryptophan in protein for the sensing of organic molecules, partial accessibility of tryptophan – modified Stern Volmer plot, study of different folding states. Protein – surfactant interaction. Excimers and exciplexes. Energy transfer: FRET, DET. Excited State Proton Transfer Preliminary ideas of absorption and fluorescence spectrophotometer.

(24 Lectures)

Nuclear Magnetic Resonance (NMR) spectroscopy

Principles of NMR spectroscopy, Larmor precession, chemical shift and low-resolution spectra, different scales, spin-spin coupling and high-resolution spectra, interpretation of PMR spectra of organic molecules.

(6 Lectures)

Electron Paramagnetic Resonance

Magnetic resonance spectroscopy – introduction, basis features of spectroscopy, Principle of EPR and comparison with NMR spectroscopy: EPR spectrometer, external standard, line width, nuclear hyper-fine splitting, anisotropy in Lande g factor, magnetically equivalent and non-equivalent set of nuclei, structural information of organic radicals and inorganic molecules (one unpaired electron), Introduction to Kramer and non-Kramer system, applications.

(14 Lectures)

Mössbauer Spectroscopy

Generation of Gamma-ray; Gamma-ray spectroscopy and its limitations; Mössbauer effect; Mössbauer spectroscopy; Basic instrumentation; Chemical shift; Splitting of Mössbauer spectra: Nuclear quadruple effect, Nuclear Zeeman effect; Spectral features of Fe-compounds in their variable oxidation and spin states; Application of Mössbauer spectra in bioinorganic systems

(8 Lectures)

Photoelectron Spectroscopies

Photoelectric effect; Koopmans' theorem; X-ray photoelectron spectroscopy (XPS); Ultraviolet photoelectron spectroscopy (UPS); Chemical shift, Spectral splitting; Applications of XPS and UPS in gases and solids

(8 Lectures)

Reference Books

- Barrow G. M. Introduction to Molecular Spectroscopy, McGraw-Hill Inc., US (1962)
- Banwell, C. N. & McCash, E. M. Fundamentals of Molecular Spectroscopy 4th Ed. Tata McGraw-Hill: New Delhi (2006).
- Kakkar, R. Atomic & Molecular Spectroscopy: Concepts & Applications, Cambridge University Press
- Lakowicz, J. R. Principles of Fluorescence Spectroscopy, 3rd edition.
- Gunther, H. NMR Spectroscopy: Basic Principle, Concepts and Applications in Chemistry - Wiley

Course Learning Outcomes: After the completion of the course, the students should be able to

1. Analyse the possible photophysical processes for electronically excited molecules
2. Explain the mode of interaction between fluorophores and quenchers which may be useful to develop the idea of optical sensing.
3. Explain theory and instrumentation of magnetic spectroscopy and its application for chemical analysis.
4. Analyse Mössbauer spectra for bioinorganic systems containing Fe in their variable oxidation states.
5. Analyse the EPR spectra of systems having unpaired electrons.

CHEM402C17: Advanced Physical Chemistry

(Credits: Theory-04, 60 Lectures, Full Marks: 50)

Course Objectives: To impart knowledge on the approximation methods in quantum chemistry, atomic spectra, ionic atmosphere, electrode kinetics and stochastic chemical kinetics.

Quantum Chemistry-III

Introduction to Classical equation of motion (forms), Heisenberg equation of motion, constant of motion, Ehrenfest's theorem. Commutator and relationship with Poisson bracket, non-compatibility and uncertainty; Formal derivation of Heisenberg uncertainty principle: commutability and compatibility.

Setting up of Schrödinger equation for many-electron atoms (He, Li). Need for approximation methods. Perturbation theory (PT) – Rayleigh-Schrödinger PT for non-degenerate states theorem, First order and second order correction in energy, First order correction to wave function, some simple applications: Anharmonic Oscillator, Ground state of helium atom

Variation method – Euler variation, principle and Rayleigh-Ritz variation theorem, application to simple systems (particle-in-a-box, harmonic oscillator, hydrogen atom). Variational treatment of helium atom, Linear variational principle, Hückel Molecular Orbital theory for π-conjugated system.

Chemical bonding: Covalent bonding, valence bond and molecular orbital approaches, LCAO-MO treatment of H_2^+. Bonding and antibonding orbitals. Qualitative extension to H_2. Comparison of LCAO-MO and VB treatments of H_2 (only wavefunctions, detailed solution not required) and their limitations. Refinements of the two approaches (Configuration Interaction for MO, ionic terms in VB). Qualitative description of LCAO-MO treatment of homonuclear diatomic molecules.

(20 Lectures)

Atomic Structure

Motion of angular momentum under magnetic field. Larmor precision. Stern Gerlach experiment. Spin-orbit interaction, conservation of total angular momentum J, Zeeman effect: Normal and Anomalous.

Motion under central force: Conservation of angular momentum and its consequence. Shape of different orbits, separation of radial and angular part. Shape of orbitals

(10 Lectures)

Electrochemistry-II

Debye-Hückel theory of strong electrolytes, concept of ionic atmosphere. Debye-Hückel limiting law for single ionic activity coefficient and mean activity coefficient (with derivation), its relation to ionic strength. Bjerrum model for ion association: Formation of ion pairs, derivation of ion- association constant.

(10 Lectures)

Kinetics II

Fast reaction - relaxation methods. Branching chain reactions and explosion. Oscillatory reactions: Lotka-Volterra model and its applications. Autocatalysis. Rate equation for electrode process. Butler-Volmer equation, High Field approximation, Tafel equation, Low field approximation, kinetic derivation of Nernst equation, exchange current density and polarizability of interfaces, concept of overvoltage.

(12 Lectures)

Stochastic Chemical Kinetics

Stochastic processes, Stochasticity in chemical reactions, Deterministic vs stochastic kinetics, Parameters of interest in stochastic kinetics, Chemical master equation (CME), Solution of CME: Generating function method, Gillespie's algorithm. Applications in enzyme kinetics and nanocatalysis.

(8 Lectures)

Reference Books

- Levine. I. N., Quantum Chemistry 7th Ed. Pearson (2016)
- Lowe, J. P. & Peterson, K. Quantum Chemistry, Academic Press (2005)
- Engel, T. & Reid, P. Physical Chemistry 3rd Ed. Pearson (2013).
- Bockris J. O. M and Reddy A. K. N., Modern Electrochemistry 1
- Glasstone S., An Introduction to Electrochemistry
- Glasstone S., Textbook of Physical Chemistry
- Laidler K. J., Chemical Kinetics
- Kapoor K. L., Physical Chemistry
- Castellan G. W., Physical Chemistry
- C. W. Gardiner C. W., Handbook of Stochastic Methods for Physics, Chemistry and Natural Sciences, Springer-Verlag: Berlin, Germany, 2004.
- Van Kampen N. G. Stochastic Processes in Physics and Chemistry, Elsevier: New York, 2007.
- Xu W., Zhang Y. and Chen T., Single Particle Nanocatalysis: Fundamentals and Applications, Wiley-VCH: Germany, 2019.

Course Learning Outcomes: After the completion of the course, the students should be able to

1. Apply various approximation methods to solve Schrodinger equation in presence of small perturbation and for multielectronic system.
2. Explain the idea of spin quantum number via Stern-Gerlach experiment, effect of magnetic field to atomic spectra and idea of the shape of the orbits and orbitals.
3. Describe the activity coefficients of electrolyte solution as a function of concentration.
4. Evaluate the ion-association constants of in solutions of weak electrolytes, and estimate the extent of associated ions.
5. Explain the kinetics of branching chain reactions and oscillatory reactions.
6. Apply the concepts of stochasticity in chemical reaction.

CHEM403C18: ORGANIC CHEMISTRY-VI

(Credits: Theory-04, 60 Lectures, Full Marks: 50)

Course Objectives: This course aims to impart knowledge on (i) Conformational aspects of alicyclic compounds and its implication in several organic reactions, (ii) Mass and ^{13}C NMR spectroscopic techniques and their applications in chemistry, (iii) Basics of photochemical reactions involving free radicals, (iv) Asymmetric synthesis and (v) Chemistry of organo-Si, Cd, Ti, and Pd.

Stereochemistry

Static Aspects: Baeyer Strain theory, Configuration – acyclic and cyclic systems, conformation – cyclic systems (cyclohexene, cyclohexanone, substituted cyclopentanes and cyclopentanones, medium rings, decalin and hydrindane systems).

Dynamic Aspects: Cyclisation reactions, Thermodynamic and kinetic control, Thorpe-Ingold effect, Baldwin's rules. Conformation and reactivity with reference to substitution, elimination, addition, and rearrangement reactions. **(16 Lectures)**

Spectroscopy

***^{13}C NMR Spectroscopy*:** Introduction, rules for ^{13}C calculations, Principles of Decoupling, NOE, relaxation processes, DEPT, Structural applications of ^{13}C NMR.

***Mass Spectrometry*:** Principles, Isotope abundances, Molecular ion, Metastable ions, Ionization Techniques (EI, CI, FD and FAB, ESI and MALDI). Fragmentation and fragmentations associated with functional groups. Applications of mass spectroscopy to simple structural and mechanistic problems. **(16 Lectures)**

Elementary idea of Free radical and Organic Photochemistry

Free Radical Reactions: Method of generation, Stability, Radical initiators, Substitution, Addition and Rearrangement reactions involving radicals.

Photochemistry of Organic Compounds and Photochemical Reactions: Basic principles, Jablonski diagram, Photoreactions of carbonyl compounds and alkenes.

(10 Lectures)

Asymmetric Synthesis

Stereoselective and Stereospecific reactions, Diastereoselectivity, and enantioselectivity, Diastereoselectivity – addition of nucleophiles to C=O adjacent to a stereogenic centre (Felkin-

Anh model), Addition of electrophiles to C=C (Houk model).

(8 Lectures)

Organometallics

Preparation and Application of organo-Si, Cd, Ti, Pd etc. C–C coupling reactions (Heck, Suzuki, Stille, etc.). **(10 Lectures)**

References Books:

- Sengupta, S. *Basic Stereochemistry of Organic Molecules*, 2nd Ed., Oxford University Press (2018).
- Nasipuri, D. *Stereochemistry of Organic Compounds*, 4th Ed., New Age International Publishers, (2020).
- Eliel, E. L. *Stereochemistry of Organic Compounds*, Wiley (2008).
- Clayden, J.; Greeves, N.; Warren, S. & Wothers, P. *Organic Chemistry*, 2nd Ed., Oxford University Press (2012).
- Kemp, W. *Organic Spectroscopy*, 3rd Ed., Macmillan (2019).
- Silverstein, R. M. *Spectrometric Identification of Organic Compounds*, 8th Ed., John Wiley & Sons Inc. (2014).
- Günther, H. *NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry*, 3rd Ed., Wiley (2013).
- Coxon, J. M. & Halton, B. *Organic Photochemistry*, 2nd Ed., Cambridge India (2015).
- Crabtree, R. H. *The Organometallic Chemistry of the Transition Metals*, 6th Ed., Wiley-Blackwell (2014).
- Elias, A. & Gupta, B. D. *Basic Organometallic Chemistry*, 2nd Ed., Universities Press (2013).

Course Learning Outcomes: After completion of the course, the student should be able to

1. Improve their basic ideas of stereochemistry related to small-large ring systems and their implication in organic synthesis.
2. Explore the theories behind ^{13}C NMR, and Mass spectrometry to realize the spectra and characterize simple/complex organic molecules.
3. Explain organic photochemical reactions with free radicals and direct metal-carbon bond and related reactions.

CHEM441C19: Project Dissertation

(Credits: 04, Full Marks: 50)

Course Objective: To provide training for literature survey, experimental and theoretical research work, instrumental techniques, and their operational procedure useful for their employability in industry and academia to orient them for future PhD programs.

Project dissertation.

The students will be carrying out a project work of 1 year duration in any of the research laboratory in the Department of chemistry according to their interest and availability of the position. This dissertation has to be submitted in the form of a thesis. The B. S. thesis will have two chapters. The chapter 1 will contain detail literature survey on the project topic and chapter 2 will contain the origin of the project work, methodology, results and discussion and conclusions. The training and the B. S. thesis of these students will then be evaluated.

Course learning outcomes: On completion of the course, the students should be able to

1. Explore new areas of research in both chemistry and allied fields of science and technology
2. Perform literature survey for the research topic of his/her area of expertise.
3. Rationalize the research gap for innovation.
4. Comprehend expertise for writing the research reports.
5. Expose safe laboratory practices by handling high end equipment and chemical reagents.

CHEM442MC05: Research Methodology

(Credits: Theory-04, 60 Lectures, Full Marks: 50)

Course Objectives: This course aims to provide knowledge on selection of research field, recent trends in research field, literature survey, lab safety, research ethics and copy right, etc.

Introduction to the concept of research: Objective of scientific research, classification of research, Identification and selection of research problem, theoretical design of methodology, diagnostic study, evaluation of research. Introduction to recent trending research topics in chemistry.

Literature survey: Need for literature survey, Sources of literature such as hardcopies and archives from university and national libraries, web sources, e-journals, e-books, search engines, identification of problem-based literature,

Basic knowledge of computer systems: writing abstract and literature-based review on word, general awareness of software packages used in research.

Basic laboratory safety protocols, Chemical safety data, chemical storage, ethical handling of chemicals, emergency procedure and first aid, concepts of drying of solvents, handling of flammable and explosive compounds disposal of laboratory chemical wastes, recovery and reuse, acquaintance of experimental setup. Use of spectroscopy and spectrometry in research.

Information about common ethical issues, copyright, intellectual property rights, citation, acknowledgement.

Reference Books,

- Garg, B. L. Karadia, R. Agarwal, F, and Agarwal, U.K. 2002, An introduction to Research Methodology, RBSA Publishers.
- Chemical Safety Matters-IUPAC-IPCS, Cambridge Univ. Press.

Course Learning Outcomes: After the completion of the course, the students should be able to

1. Select and approach the research problems
2. Perform literature survey on particular research topic
3. Write the abstract, literature survey outcomes etc.
4. Follow basic lab safety protocols and handling of hazardous chemicals, first aid
5. Analyse the spectroscopy and spectrometry data
6. Follow ethics in research, copyright and citation

SEMESTER- VIII

CHEM451C20: Soft Materials Nanomaterials and Advanced Functional Materials

(Credits: Theory-04, 60 Lectures, Full Marks: 50)

Course Objectives: To impart knowledge on adsorption isotherms, soft matter chemistry functional nanomaterials, energy storage materials and fundamental of characterization techniques

Soft Materials

Introduction to soft materials / soft matter; unifying features of soft materials; Brownian motion and diffusion in connection with the study of soft materials – the Stokes-Einstein relation; basic concepts of rheology.

(4 Lectures)

Polymers

Introduction to polymers; ideal and Flory chains; the theta temperature and coil-globule transitions; viscoelasticity of polymers; determination of molecular weights of polymers by different experimental techniques.

(6 Lectures)

Surfactants Surface tension, adsorption, surface excess and surfactants; different types of surfactants; self-assembled structures; phase diagrams.

(6 Lectures)

Colloids

Stability of colloidal suspensions – the DLVO theory; colloidal interactions; engineering phase behaviour; thermodynamics and kinetics of phase transitions in certain colloidal model systems.

(6 Lectures)

Liquid Crystals

Introduction to mesophases; concepts of order parameters; theories of phase transitions in the context of liquid crystals; experimental techniques in characterising mesophases and phase transitions in liquid crystals; basics of liquid crystal displays.

(6 Lectures)

Nanomaterials and Advanced functional Materials

Fundamentals of nano science: definition, nano versus bulk, quantum confinement: nanoscale in 1D, 2D and 3D with examples, synthesis of nano materials: top-down and bottom-up approaches, size and shape dependent optical properties of semiconductive (CdSe) and

plasmonic metal nanoparticles, nanoclusters and nanowires, nanoparticles, concept of magnetic nanoparticles, applications of nanomaterials.

(5 Lectures)

Characterization of Nanomaterials

Introduction to surface spectroscopy, Microscopy, problems of surface analysis, Fundamental principles, Instrumentation and applications: Fourier-transform infrared spectroscopy, Brunauer-Emmett-Teller (BET) surface area, X-ray photoelectron spectroscopy (XPS), X-ray powder diffraction, Transmission electron microscopy image, Scanning electron microscopy (SEM), Atomic Force Microscopy (AFM), Energy dispersive X-ray spectroscopy (EDS), Temperature programmed desorption, Temperature programmed reduction (TPR), Secondary Ion Mass Spectroscopy (SIMS).

(7 Lectures)

Novel Inorganic Materials

Fundamentals of inorganic solids, brief introduction to self-assembled nanostructures, inorganic-organic hybrid, Inorganic pigments, One-dimensional metals, inorganic liquid crystals, metal oxide nanoparticles, semiconducting oxides and its applications. Synthesis of Inorganic solids: Conventional heat and beat methods, co-precipitation methods, sol-gel methods, hydrothermal method, Ceramic method, microwave synthesis, Chemical vapor deposition (CVD), Ion-exchange method and Intercalation method.

(10 Lectures)

Energy Storage Materials

Significance of electrochemical energy storage, Classifications of energy storage devices-batteries and supercapacitors; Energy storage mechanisms; Materials design for energy storage; Cyclic Voltammetric, electrochemical impedance spectroscopic and chronopotentiometric characterizations for energy storage materials; Classification of batteries-primary and secondary; Mechanisms of lead-acid and lithium-ion batteries; Classifications of supercapacitors; Electrical double layer capacitors; pseudocapacitors; hybrid capacitors; Futuristic materials for battery and supercapacitor applications.

(10 Lectures)

Reference Books

- Billmeyer, Jr Fred W. Textbook of Polymer Science, 3rd Ed., John Wiley & Sons (1984).
- Odian, G. Principles of Polymerization 1st Ed., John Wiley & Sons, Inc. (2004).
- Castellan, G. W. Physical Chemistry 4th Ed., Narosa (2004).

- Das A.K., Das Mahua, An Introduction to Nanomaterials and Nanoscience, CBS publishers and distributors Pvt Ltd (2019).
- Rakshit, P. C. Physical Chemistry, 7th Ed., Sarat Book House (2014).
- Munaweera I., Chamalki Madhusha, M.L. Characterization Techniques for Nanomaterials. 7th Ed., CRC Press (2023).
- Electrochemical Supercapacitors: Scientific Fundamentals and Technological Applications by B. E. Conway
- Lithium-Ion Batteries: Science and Technologies by M. Yoshio, R. J. Brodd and A. Kozawa
- Lead-Acid Batteries: Science and Technology by D. Pavlov

Course Learning Outcomes: After the completion of the course, the students should be able to

1. Explain the isotherms empirically as well as molecular basis, chemistry of surfactants, and surface excess.
2. Derive various molecular weight of polymers, explain polydispersity and crystallinity in polymer system.
3. Describe the origin properties of colloidal sol, stability of particles.
4. Classify colloidal particle according to dimensions and applications.
5. Identify the appropriate materials of batteries and supercapacitors for targeted applications.
6. Get specific idea about synthesis functional materials and basics of characterization techniques.

CHEM452C21: INORGANIC CHEMISTRY-VI

(Credits: Theory-04, 60 Lectures, Full Marks: 50)

Course Objectives: The course aims to provide the knowledge on chemical equilibrium, kinetics, reaction & mechanism of inorganic complexes. Also aims to introduce the structure and bonding of inorganic clusters, compare the structure with organic analogue using isolobal principle. To impart the knowledge of spectroscopic analysis for inorganic systems.

Chemistry of Complex Equilibria:

Trans-Effect, uses of Trans-Effect, theories of Trans-Effect, Kinetic-, thermodynamic stability of metal complexes. Statistical and non- statistical factors influencing stability of complexes in solution, stability and reactivity of mixed ligand complexes. Determination of composition and stability constants of complexes by continuous variation method, spectrophotometric and potentiometric methods. Alkali metal complexes with macrocyclic ligands, crown ether and cryptate complexes. **(10 Lectures)**

Inorganic Reaction Kinetics and Mechanism

Introduction to inorganic reaction mechanisms, Substitution reactions: Four board classes of mechanism of substitution – 'D', 'A', 'Ia' and 'Id'; Solvent exchange, Aquation, Anation, Base hydrolysis, pseudo-substitution; Mechanism of isomerisation and racemisation reactions: Linkage isomerism, Cis-Trans isomerism, Intramolecular and intermolecular racemisation, Ray– Dutta and Bailar twist mechanisms; Mechanism of electron transfer reactions: General characteristics and classification of redox reactions, self-exchange reactions, Net redox reactions, Outer sphere and inner sphere reactions, Applications of Marcus expression (simple form), Redox catalysed substitution reactions; Inorganic photochemistry **(16 Lectures)**

Inorganic Cages & Clusters

Structure and bonding of higher boranes, carboranes, metallocarboranes, Lipscomb's tropological diagrams and Wade's rules. Metal Clusters (low and high nuclearity carbonyl clusters), Skeletal electron counting, Wade-Mingos rule, application of iso electronic and isolobal relationships and caping rules. Metal-metal bonded complexes of metals (structure and bonding): dirhenium complexes. **(10 Lectures)**

Advanced Spectroscopy for Inorganic Compounds

Electronic Spectroscopy: Laporte and spin election rules; Relaxation of Laporte selection rules: Vibronic coupling, d-p mixing; Lowering of the symmetry; Relaxation of spin selection rules: Spin orbit coupling; Term symbol for different d^n configurations; Racah parameters, Nephelauxetic effect; Free ion terms and their splitting in O_h and T_d symmetry; Correlation between weak and strong field terms, Correlation table; Limitations of Orgel diagrams, Introduction of Tanabe Sugano diagrams; Bonding parameters and structural evidences from electronic spectra of d-metal complexes, Electronic spectra of lanthanides and actinides

IR and Raman Spectroscopy: Dipole moment; Polarizability; Symmetry of normal modes; Mutual exclusion principle; Structure determination from combined IR and Raman spectroscopy

NMR spectra: ^{11}B, ^{13}C, ^{19}F, ^{27}Al, ^{31}P NMR spectroscopy with typical examples, ^{1}HNMR spectra of coordination compounds of paramagnetic metal ions, dipolar and contact shifts, magnetic susceptibility and **resonance shift.**

NQR spectroscopy: Principle, nuclear quadruple coupling constants, structural information from NQR spectra. **(24 Lectures)**

Reference Books:

- Huheey, J. E.; Keiter, E.A. & Keiter, R.L. Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed., Harper Collins 1993, Pearson,2006
- Selected Topics in Inorganic Chemistry - W. U. Malik, G. D. Tuli, R. D. Madan
- A. Elias, B. D. Gupta, Basic Organometallic Chemistry, Universities Press (ed. 2), 2013.
- Miessler, G. L. & Tarr, D.A. Inorganic Chemistry 4th Ed., Pearson, 2010.
- Purcell, K.F & Kotz, J.C. Inorganic Chemistry W.B. Saunders Co, 1977.
- Inorganic Spectroscopic Methods - Alan K Brisdon.
- Physical Methods for Chemists - R. S. Drago.
- Fundamentals of Molecular spectroscopy - N. Banwell, E. M. McCash.

Course Learning Outcomes: On completion of the course, the students should be able to

1. Determine the chemical composition and ligand lability properties using different techniques.
2. Structure and bonding of boranes, carbonyls and other metal clusters using Lipscomb topological approach, Wade's rule and isolobal analogy.
3. Explain the mechanistic pathway of inorganic reactions for coordination compounds
4. Rationalize the spectral properties of inorganic materials with appropriate theory

CHEM453C22: Organic Chemistry-VII

(Credits: Theory-04, 60 Lectures, Full Marks: 50)

Course Objectives: This course aims to impart advanced knowledge on (i) application of modern B, S and Si-based reagents in multistep organic syntheses (ii) designing synthetic strategies toward complex molecular targets such as bioactive heterocycles and natural products including alkaloids, terpenoids and their stereochemistry and structure elucidation.

Synthetic methodology

Roles of Boron, Sulfur and Silicon in organic synthesis. Stereoselective Hydroboration, Hydrogenation, Epoxidation, and Hydroxylation. Application of modern reagents in organic synthesis. **(20 Lectures)**

Heterocyclic Chemistry

Systematic nomenclature (Hantzsch-Widman system) for monocycle and fused heterocycles. General approach to heterocyclic synthesis – cyclisation and cycloaddition routes. Heterocycles in organic synthesis – masked functionalities, umpolung, Stork annulation reaction and applications (synthesis of testosterone, estrone, progesterone, ranitidine, lansoprazole and recently discovered molecules). Rearrangement and ring transformation involving 5- and 6-membered heterocycles with one heteroatom.

(20 Lectures)

Natural Products

Alkaloids: Definition, Classification, Extraction, General properties and methods for structure elucidation, Hoffmann's exhaustive methylation, Emde's modification. Structure elucidation, Reactions, Stereochemistry, and Synthesis (Classical/Asymmetric) of some representative Alkaloids (Hygrine, Quinine, Morphine, Camptothecin and recently discovered bioactive natural products).

Terpenoids: Classification, Isoprene rule, Stereochemistry, Reactions, and Synthesis of Terpenoids and Carotenoids (Zingiberine, Santonin, Abietic acid, β-Carotene etc).

(20 Lectures)

Reference Books:

- Carruthers, W. & Coldham, I. *Modern Methods of Organic Synthesis*, 4th Ed., Cambridge University Press (2015).

- Clayden, J.; Greeves, N.; Warren, S. & Wothers, P. *Organic Chemistry*, 2nd Ed., Oxford University Press (2012).
- Norman, R. O. C. & Coxon, J. M. *Principle of Organic Synthesis*, 2nd Ed., Springer (1993).
- Trost, B. M. *Comprehensive Organic Synthesis*, Pergamon (1991).
- Joule, J. A. & Mills, K. *Heterocyclic Chemistry*, 5th Ed., Wiley (2010).
- Gilchrist, T. L. *Heterocyclic Chemistry*, 3rd Ed., Pearson (2005).
- Meyers, A. I. *Heterocycles in Organic Synthesis*, John Wiley & Sons Inc. (1974).
- Talapatra, S. K. *Chemistry of Plant Natural Products: Stereochemistry, Conformation, Synthesis, Biology, and Medicine*, Springer (2015).
- Finar, I. L. *Organic Chemistry, Vol. 2:Stereochemistry and the Chemistry Natural Products*, 5th Ed., Pearson (2002).

Course Learning Outcomes: After completion of the course, the student should be able to

1. Explicate the use of modern reagents and their chemistry based on boron, sulfur, and silicon.
2. Expand the knowledge of simple and complex organic molecules containing one or more heteroatom.
3. Elucidate structures, stereochemistry, various total synthetic pathways, and reactions of classical and recently discovered bioactive natural products (alkaloids, terpenoids and carotenoids).

CHEM491C23: Project Dissertation

(Credits: 08, Full Marks: 100)

Course Objective: To provide training for literature survey, experimental and theoretical research work, instrumental techniques, and their operational procedure useful for their employability in industry and academia to orient them for future PhD programs.

Project dissertation.

The students will be carrying out a project work of 1 year duration in any of the research laboratory in the Department of chemistry according to their interest and availability of the position. This dissertation has to be submitted in the form of a thesis. The B. S. thesis will have two chapters. The chapter 1 will contain detail literature survey on the project topic and chapter 2 will contain the origin of the project work, methodology, results and discussion and conclusions. The training and the B. S. thesis of these students will then be evaluated.

Course learning outcomes: On completion of the course, the students should be able to

1. Explore new areas of research in both chemistry and allied fields of science and technology
2. Perform literature survey for the research topic of his/her area of expertise.
3. Rationalize the research gap for innovation.
4. Comprehend expertise for writing the research reports.
5. Expose safe laboratory practices by handling high end equipment and chemical reagents.

CHEM492MC06: Research and Publication Ethics

(Credits: Theory-04, 60 Lectures, Full Marks: 50)

Course Objectives: To impart knowledge on the ethics of publication and research.

Philosophy and Ethics: Introduction to philosophy: definition, nature and scope, concept, branches. Ethics: definition, moral philosophy, nature of moral judgements and reactions

(8 Lectures)

Scientific Conduct: Ethics with respect to science and research. Intellectual honesty and research integrity. Scientific misconducts: Falsification, Fabrication, and Plagiarism (FFP). Redundant publications: duplicate and overlapping publications, salami slicing. Selective reporting and misrepresentation of data.

(8 Lectures)

Publication Ethics: Publication ethics: definition, introduction, and importance. Best practices /standards setting initiatives and guidelines: COPE, WAME, etc. Conflicts of interest. Publication misconduct: definition, concept, problems that lead to unethical behavior and vice versa, types. Violation of publication ethics, authorship and contributorship. Identification of publication misconduct, complaints, and appeals. Predatory publishers and journals.

(14 Lectures)

HANDS ON SESSIONS

Open Access Publishing:

1. Open access publications and initiatives
2. SHERPA/RoMEO online resource to check publisher copyright & self-archiving policies
3. Software tool to identify predatory publications developed by SPPU
4. Journal finder / journal suggestion tools viz. JANE, Elsevier Journal Finder, Springer Journal Suggester, etc.

(8 Lectures)

Publication Misconduct:

A. Group Discussions

1. Subject specific ethical issues, FFP, authorship
2. Conflicts of interest
3. Complaints and appeals: examples and fraud from India and abroad

B. Software tools

Use of plagiarism software like Turnitin, Urkund and other open source software tools

(8 Lectures)

Databases and Research Metrics:

A. Databases

1. Indexing databases
2. Citation databases: Web of Science, Scopus, etc.

B. Research Metrics

1. Impact Factor of journal as per Journal Citation Report, SNIP, SJR, IPP, Cite Score
2. Metrics: h-index, g index, i10 index, altmetrics

(14 Lectures)

Reference Books:

- Bird, A. (2006). *Philosophy of Science.* Routledge.
- Maclntyre, Alasdair (1967) *A Short History 0/ Ethics.* London.
- P. Chaddah, (2018) Ethics in Competitive Research: Do not get scooped; do not get plagiarized, ISBN:978-9387480865
- National Academy of Sciences, National Academy of Engineering and Institute of Medicine. (2009). *On Being a Scientist: A Guide to Responsible Conduct in Research: Third Edition.* National Academies Press.
- Resnik, D. B. (2011). What is ethics in research & why is it important. *National Institute of Environmental Health Sciences,* 1-10. Retrieved from https://www.niehs.nih.govlresearchlresoul'ces/bioethics/whatislindex.cfm
- Beall, J. (2012). Predatory publishers are corrupting open access. Nature, 489(7415), 179-179. https://doi.org/IO.1038/489179a.
- Indian National Science Academy (INSA), Ethics in Science Education, Research and Governance (2019), ISBN :978-81-939482-1-7.http://www.insaindia.res.inlpdf/Ethics Book.pdf

Course Learning Outcomes: After the completion of the course, the students should be able to

1. Conduct the research in an scientific and ethical manner
2. Describe and use the different indexing, citation databases and research metrics.