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B.Sc. (H) CHEMISTRY
THREE YEAR FULL TIME PROGRAMME
(Six –Semester Course)

Under
CHOICE BASED CREDIT SYSTEM



COURSE CONTENTS

Department of Chemistry
Oriental College (Autonomous)
Takyel, Imphal
AFFILIATED TO MANIPUR UNIVERSITY, CANCHIPUR

Preamble

The choice based credit system is naturally the next logical step in a credit based semester system. This makes the system the more learner-centric. A CBCS offers the student a diversity of courses to choose from and the autonomy to decide on the place, pace and the time of learning.

The Oriental College, Imphal has decided to introduce the CBCS system at the under graduate level from the session 2020-21. The CBCS syllabus for the B.Sc. (Honours) is prepared in the model of syllabus prepared by the UGC.

A student opting for honours course in chemistry must have and passed the Mathematics as a subject in the Senior Secondary level examination.

Course Structure

Course	*Credits
	Theory+ Practical
I. Core Course (14 Papers) Core Course Practical / Tutorial* (14 Papers)	14 x 4 = 56 14 x 2 = 28
II. Elective Course (8 Papers) A 1. discipline Specific Elective (4 papers) A. 2. discipline Specific Elective Practical / Tutorials*(4 papers)	4x4=16 4x 2 = 8
B.1. Generic Elective/ Interdisciplinary (4 papers) B. 2. Generic Elective practical / Tutorial* (4papers)	4 x4= 16 4 x 2 = 8
III. Ability Enhancement Courses 1. Ability Enhancement Compulsory (2 Papers of 4 credit each) Environmental Studies English/MIL Communication 2. Ability Enhancement Elective (Skill Based) (Minimum 2) (2 Papers of 4 credit each)	2x 4 = 8 2 x 4 = 8
Total	148

***Core and DSE courses without practicals will have tutorial and have credit distribution of : 5 credits for theory and 1 credit for tutorial, total 6 credits, same as the papers with practical**

STRUCTURE OF BSC HONOURS (CHEMISTRY) PROGRAMME

SEM	types	Core	AECC	SEC	DSE	GEN
	Credits	14 x 6 = 84	2 x 4 = 8	2 x 4 = 8	4 x 6 = 24	4 x 6 = 24
I	CHE-HC-1016	ENG-AE-1014				XXX-HG-1XX6
	CHE-HC-1026					
II	CHE-HC-2016	ENV-AE-2014				XXX-HG-2XX6
	CHE-HC-2026					
III	CHE-HC-3016			CHE-SE-3YY4†		XXX-HG-3XX6
	CHE-HC-3026					
	CHE-HC-3036					
IV	CHE-HC-4016			CHE-SE-4YY4†		XXX-HG-4XX6
	CHE-HC-4026					
	CHE-HC-4036					
V	CHE-HC-5016				CHE-HE-5YY5#	
	CHE-HC-5026					
VI	CHE-HC-6016				CHE-HE-6YY6#	
	CHE-HC-6016					

Abbreviation:

CHE-HC- Chemistry Honours Core Course

DSE- Discipline specific elective course

GE- Generic elective course

SEC- Skill enhancement course

AECC-Ability enhancement compulsory course

SCHEME FOR CHOICE BASED CREDIT SYSTEM IN B. Sc.

Honours (Chemistry)

SEM	COURSE OPTED	COURSE NAME	CREDITS
I	ENG-AE-1014	English Communications	4
	CHE-HC-1016	<u>Inorganic Chemistry-1</u> Inorganic Chemistry-1 Lab	4 + 2 = 6
	CHE-HC-1026	<u>Physical Chemistry-1</u> Physical Chemistry-1 Lab	4 + 2 = 6
	AAA-HG-1YY6*	<u>GE-1</u> Generic Elective-1 Practical	4 + 2 = 6
Total Credits in Semester I			22
II	Ability Enhancement Computer Course-II**	Environmental Studies	4
	CHE-HC-2016	<u>Organic Chemistry-I</u> Organic Chemistry -1 Lab	4 + 2 = 6
	CHE-HC-2026	<u>Physical Chemistry-II</u> Physical Chemistry-II Lab	4 + 2 = 6
	AAA-HG-2YY6*	<u>GE-2</u> Generic Elective-2 Practical	4 + 2 = 6
Total Credits in Semester II			22
III	CHE-HC-3016	<u>Inorganic Chemistry-II</u> Inorganic Chemistry-II Lab	4 + 2 = 6
	CHE-HC-3026	<u>Organic Chemistry-II</u> Organic Chemistry –II Lab	4+2 = 6
	CHE-HC-3036	<u>Physical Chemistry-III</u> Physical Chemistry-III Lab	4 + 2 = 6
	CHE-SE-3YY4†	SEC-1	4
	AAA-HG-3YY6*	<u>GE-3</u> Generic Elective-3 Practical	4 + 2 = 6
Total Credits in Semester III			28
IV	CHE-HC-4016	<u>Inorganic Chemistry-III</u> Inorganic Chemistry-III Lab	4 + 2 = 6
	CHE-HC-4026	<u>Organic Chemistry-III</u> Organic Chemistry –III Lab	4+2=6
	CHE-HC-4036	<u>Physical Chemistry-IV</u> Physical Chemistry-IV Lab	4 + 2 = 6
	CHE-SE-4YY4 †	SEC-2	4
	AAA-HG-4YY6*	<u>GE-4</u> Generic Elective-4 Practical	4 + 2 = 6
Total Credits in Semester IV			28
V	CHE-HC-5016	<u>Organic Chemistry-IV</u> Organic Chemistry –IV Lab	4+ 2 = 6
	CHE-HC-5026	<u>Physical Chemistry-V</u> Physical Chemistry-V Lab	4+ 2 = 6

	CHE-HE-5YY6†	DSE-1	4+ 2 =6
		DSE-1 Lab	
	CHE-HE-5YY6†	DSE-2	4+ 2 =6
		DSE-2 Lab	
Total Credits in Semester V			24
VI	CHE-HC-6016	Inorganic Chemistry-IV	4 + 2 =6
		Inorganic Chemistry-IV Lab	
	CHE-HC-6026	Organic Chemistry-V	4 + 2 =6
		Organic Chemistry –V Lab	
	CHE-HE-6YY6†	DSE-3	4 + 2 =6
		DSE-3 Lab	
	CHE-HE-6YY6†	DSE-4	4 + 2 =6
		DSE-3 Lab	
Total Credits in Semester VI			24
Grand Total Credits			148

‡ **Discipline Specific Elective Papers: (Credit: 06 each) (4 papers to be selected)-**
DSE for Semester V

DSE-1(Any One from the following)

1. **CHE-HE-5016:** Applications of Computers in Chemistry (4) + Lab (2)
2. **CHE-HE-5026:** Analytical Methods in Chemistry (4) + Lab (2)
3. **CHE-HE-5036:** Molecular Modelling & Drug Design (4) + Lab (2)

DSE-2(Any One from the following)

4. **CHE-HE-5046:** Novel Inorganic Solids (4) + Lab (2)
5. **CHE-HE-5056:** Polymer Chemistry (4) + Lab (2)
6. **CHE-HE-5066:** Instrumental Methods of Analysis (4) + Lab (2)

DSE for Semester VI

DSE-3(Any One from the following)

7. **CHE-HE-6016:** Green Chemistry (4) + Lab (2)
8. **CHE-HE-6026:** Industrial Chemicals & Environment (4) + Lab (2)
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9. **CHE-HE-6036:** Inorganic Materials of Industrial Importance (4) + Lab (2)

DSE-4(Any One from the following)

10. **CHE-HE-6046:** Research Methodology for Chemistry (5) + Tutorials (1)
11. **CHE-HE-6056:** Dissertation

† **Skill Enhancement Courses (04 papers) (Credit: 04 each)**

SEC for Semester III

Any One from the following

1. **AAA-SE-3014 :** English (Syllabus to be included as and when available)
2. **CHE-SE-3024:** IT Skills for Chemists
3. **CHE-SE-3034:** Basic Analytical Chemistry
4. **CHE-SE-3044:** Chemical Technology & Society
5. **CHE-SE-3054:** Chemoinformatics
6. **CHE-SE-3064:** Business Skills for Chemists
7. **CHE-SE-3074:** Intellectual Property Rights

SEC for Semester IV

Any One from the following

8. **CHE-SE-4014:** Analytical Clinical Biochemistry
9. **CHE-SE-4024:** Green Methods in Chemistry
10. **CHE-SE-4034:** Pharmaceutical Chemistry
11. **CHE-SE-4044:** Chemistry of Cosmetics & Perfumes
12. **CHE-SE-4054:** Pesticide Chemistry

13. CHE-SE-4064: Fuel Chemistry

****Ability Enhancement Compulsory Courses (02 papers) (Credit: 04 each)**

AECC for Semester I

1. ENG-AE-1014: English Communications

AECC for Semester II

2. ENV-AE-2014: Environmental Science

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CORE COURSE (HONOURS IN CHEMISTRY)

Semester I

CHE-HC-1016: INORGANIC CHEMISTRY-I

(Credits: Theory-04, Practicals-02)

Course Objectives: This course aims at giving students theoretical understanding about the basic constituents of matter – atoms, ions and molecules in terms of their electronic structure and reactivity. Structure and bonding in/of these are to be dealt with basic quantum chemistry treatment. Reactivity of chemical species based on their electron transfer affinity is introduced. Further, periodic classification of elements in the periodic table and changes in properties along the periods and groups to be studied in detail. Accompanying laboratory course is designed for students to have hands-on experience of basic quantitative analytical techniques related to volumetric titrations.

Learning Outcome: On successful completion, students would have clear understanding of the concepts related to atomic and molecular structure, chemical bonding, periodic properties and redox behaviour of chemical species. Students will also have hands on experience of standard solution preparation in different concentration units and learn volumetric estimation through acid-base and redox reactions.

Atomic Structure:

Bohr's theory, its limitations and atomic spectrum of hydrogen atom. Wave mechanics de-Broglie equation, Heisenberg's uncertainty principle and its significance, Schrodinger wave equation, significance of Ψ and Ψ^2 , radial and angular wave functions, and probability distribution curves, shapes of s, p, and d orbitals, quantum numbers and their significance, Pauli's Exclusion Principle, Hund's rule of maximum multiplicity, aufbau's principle and its limitations, variation of energy of atomic orbitals with atomic number.

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 & p-block.

- Effective nuclear charge, shielding or screening effect, Slater rules, variation of effective nuclear charge in periodic table.
- Atomic radii (van der Waals)
- Ionic and crystal radii.
- Covalent radii (octahedral and tetrahedral)
- Ionization enthalpy, Successive ionization enthalpies and factors affecting ionization energy. Applications of ionization enthalpy.
- Electron gain enthalpy, trends of electron gain enthalpy.
- 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. Sanderson's electron density ratio.

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). Energetics of 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 , and their ions; 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 rules 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.

(iv) *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, solubility energetics of dissolution process.

Oxidation-Reduction:

Redox equations, Standard Electrode Potential and its application to inorganic reactions.

Principles involved in volumetric analysis to be carried out in class.

Recommended Books:

1. Lee, J. D. Concise Inorganic Chemistry, 5th Ed., Oxford University Press, 2008.
2. Douglas, B.E. and Mc Daniel, D.H., Concepts and Models of Inorganic Chemistry, 3rd Ed. Wiley India, 2006.
3. Cotton, F.A., Wilkinson, G. and Gaus, P. L., Basic Inorganic Chemistry, 3rd Ed., Wiley, 2007.
4. Cotton, F.A. & Wilkinson, G, Advanced Inorganic Chemistry. 6th Ed., Wiley-VCH, 2007.
5. Atkins, P.W. & Paula, J. Physical Chemistry, 11th Ed., Oxford University Press, 2018.
6. Housecroft, C. E. and Sharpe, A. G. Inorganic Chemistry, 5th Ed., Pearson, 2018.
7. Day, M.C. and Selbin, J. Theoretical Inorganic Chemistry, Literary Licensing, LLC, 2012.

CHE-HC-1016: LAB

(A) Titrimetric Analysis

- (i) Calibration and use of common laboratory apparatus
- (ii) Preparation of solutions of different Molarity/Normality of titrants

(B) Acid-Base Titrations

- (i) Estimation of carbonate and hydroxide present together in mixture.
- (ii) Estimation of carbonate and bicarbonate present together in a mixture.
- (iii) Estimation of free alkali present in different soaps/detergents

(C) Oxidation-Reduction Titrimetry

- (i) Estimation of Fe(II) and oxalic acid using standardized $KMnO_4$ solution.
- (ii) Estimation of oxalic acid and sodium oxalate in a given mixture.

(ii) Estimation of Fe(II) with $K_2Cr_2O_7$ using internal (diphenylamine, anthranilic acid) and external indicator.

Recommended Books:

1. Mendham, J. et al.: Vogel's Text Book of Quantitative Chemical Analysis; 6th Ed. Pearson Education, 2009.

CHE-HC-1026: PHYSICAL CHEMISTRY I

(Credits: Theory-04, Practicals-02)

Course objective: This course contains states of matter- gaseous, liquid and solid states along with ionic equilibria. A small unit of molecular and crystal symmetry is also there in the course.

Learning outcome: In gaseous state unit the students will learn the kinetic theory of gases, ideal gas and real gases. In liquid state unit, the students are expected to learn the qualitative treatment of the structure of liquid along with the physical properties of liquid, viz, vapour pressure, surface tension and viscosity. In the molecular and crystal symmetry unit they will be introduced to the elementary idea of symmetry which will be useful to understand solid state chemistry and group theory in some higher courses. In solid state unit the students will learn the basic solid state chemistry application of x-ray crystallography for the determination of some very simple crystal structures. The students will also learn another important topic "ionic equilibria" in this course.

Gaseous state:

Kinetic molecular model of a gas: postulates and derivation of the kinetic gas equation; 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. Maxwell distribution and its use in evaluating molecular velocities (average, root meansquare and most probable) and average kinetic energy.

Behaviour of real gases: Deviations from ideal gas behaviour, 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.

Liquid state:

Qualitative treatment of the structure of the liquid state; Radial distribution function; physical properties of liquids; vapour pressure, surface tension and coefficient of viscosity, and their determination. Effect of addition of various solutes on surface tension and viscosity.

Explanation of cleansing action of detergents. Temperature variation of viscosity of liquids and comparison with that of gases.

Qualitative discussion of structure of water.

Molecular and Crystal Symmetry

Elementary ideas of symmetry, symmetry elements and symmetry operations, qualitative idea

of point and space groups, seven crystal systems and fourteen Bravais lattices.

Solid state:

Nature of the solid state, law of constancy of interfacial angles, law of rational indices, Miller indices; 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. Liquid crystals (Introductory idea)

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; 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.

Multistage equilibria in polyelectrolyte systems; hydrolysis and hydrolysis constants.

Recommended Books:

1. Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry Ed., Oxford University Press (2006).
2. Ball, D. W. Physical Chemistry Thomson Press, India (2007).
3. Castellan, G. W. Physical Chemistry 4th Ed. Narosa (2004).
4. Mortimer, R. G. Physical Chemistry 3rd Ed. Elsevier: NOIDA, UP (2009).
5. Puri, B. R.; Sharma, L. R.; Pathania, M. S. Principles of Physical Chemistry, Vishal Publishing Co. (2017)
6. Kapoor, K. L. A Textbook of Physical Chemistry (Volume 1) McGraw Hill Education; Sixth edition (2019)

CHE-HC-1026: LAB

1. Surface tension measurements.

- a. Determine the surface tension by (i) drop number (ii) drop weight method.
- b. Study the variation of surface tension of detergent solutions with concentration.

2. 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.

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

4. pH metry

- a. Study the effect on pH of addition of HCl/NaOH to solutions of acetic acid, sodium acetate and their mixtures.
- b. Preparation of buffer solutions of different pH
 - i. Sodium acetate-acetic acid
 - ii. Ammonium chloride-ammonium hydroxide
- c. pH metric titration of (i) strong acid vs. strong base, (ii) weak acid vs. strong base.

d. Determination of dissociation constant of a weak acid.

Recommended Books

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

Semester II

CHE-HC-2016: ORGANIC CHEMISTRY I

(Credits: Theory-04, Practicals-02)

Course Objectives: This course is inducted to apprise students with introduction to organic compounds, electron displacement, type of reagents and reaction intermediates. The chemistry of aliphatic and aromatic hydrocarbon, conformational analysis of cycloalkanes and basic stereochemical phenomena are included.

Students are expected to learn different classes learn, explain, describe and analyze different classes of organic compounds, their reactivities and mechanisms along with stereo chemical considerations.

Learning Outcome: Students will be able to identify different classes of organic compounds, describe their reactivity and explain/analyze their chemical and stereo chemical aspects.

Basics of Organic Chemistry

Organic Compounds: Classification, and Nomenclature, Hybridization, Shapes of molecules, Influence of hybridization on bond properties.

Electronic Displacements: Inductive, electromeric, resonance and mesomeric effects, hyperconjugation and their applications; Dipole moment; Organic acids and bases; their relative strength.

Homolytic and Heterolytic fission with suitable examples. Curly arrow rules, formal charges; Electrophiles and Nucleophiles; Nucleophilicity and basicity; Types, shape and their relative stability of Carbocations, Carbanions, Free radicals and Carbenes.

Introduction to types of organic reactions and their mechanism: Addition, Elimination and Substitution reactions.

Stereochemistry:

Fischer Projection, Newmann and Sawhorse Projection formulae and their interconversions; Geometrical isomerism: cis–trans and, syn-anti isomerism E/Z notations with C.I.P rules.

Optical Isomerism: Optical Activity, Specific Rotation, Chirality/Asymmetry, Enantiomers, Molecules with two or more chiral-centres, Distereoisomers, meso structures, Racemic mixture and resolution. Relative and absolute configuration: D/L and R/S designations.

Chemistry of Aliphatic Hydrocarbons

A. Carbon-Carbon sigma bonds

Chemistry of alkanes: Formation of alkanes, Wurtz Reaction, Wurtz-Fittig Reactions, Free radical substitutions: Halogenation -relative reactivity and selectivity.

B. Carbon-Carbon pi bonds:

Formation of alkenes and alkynes by elimination reactions, Mechanism of E1, E2, E1cb reactions. Saytzeff and Hofmann eliminations.

Reactions of alkenes: Electrophilic additions and their mechanisms (Markownikoff/ Anti Markownikoff addition), mechanism of oxymercuration-demercuration, hydroborationoxidation, ozonolysis, reduction (catalytic and chemical), syn and antihydroxylation (oxidation). 1,2- and 1,4-addition reactions in conjugated dienes and, Diels-Alder reaction; Allylic and benzylic bromination and mechanism, e.g. propene, 1-butene, toluene, ethyl benzene.

Reactions of alkynes: Acidity, Electrophilic and Nucleophilic additions. Hydration to form carbonyl compounds, Alkylation of terminal alkynes.

C. Cycloalkanes and Conformational Analysis

Types of cycloalkanes and their relative stability, Baeyer strain theory, Conformation analysis of alkanes: Relative stability: Energy diagrams of cyclohexane: Chair, Boat and Twist boat forms; Relative stability with energy diagrams.

Aromatic Hydrocarbons

Aromaticity: Hückel's rule, aromatic character of arenes, cyclic carbocations/carbanions and heterocyclic compounds with suitable examples. Electrophilic aromatic substitution: halogenation, nitration, sulphonation and Friedel-Craft's alkylation/acylation with their mechanism. Directing effects of the groups.

Recommended Books:

1. Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Finar, I. L. *Organic Chemistry* (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
3. Eliel, E. L. & Wilen, S. H. *Stereochemistry of Organic Compounds*, Wiley: London, 1994.
4. Nasipuri, D. *Stereochemistry of Organic Compounds*, Wiley Eastern Limited.
5. Kalsi, P. S. *Stereochemistry Conformation and Mechanism*, New Age International, 2005.
6. Subrata Sen Gupta, *Basic Stereochemistry of Organic Molecules*, Oxford Higher Education.
7. Dhillon, R. S.; Singh, I. P. & Baskar, C. *Stereochemistry*, Narosa.
8. Loudon, G. M. *Organic Chemistry*, Oxford.
9. Sykes, P. *A guidebook to Mechanism in Organic Chemistry*, Pearson Education, 2003.
10. Clayden, J., Greeves, N. & Warren, S. *Organic Chemistry*, Second edition, Oxford University Press, 2012.

CHE-HC-2016: LAB

60 Lectures

1. Checking the calibration of the thermometer
2. Purification of organic compounds by crystallization using the following solvents:
 - a. Water
 - b. Alcohol
 - c. Alcohol-Water
3. Determination of the melting points of above compounds and unknown organic Compounds.

4. Effect of impurities on the melting point – mixed melting point of two unknown organic Compounds.
5. Determination of boiling point of liquid compounds. (boiling point lower than and more than 100 °C by distillation and use of thiele tube method)
6. Chromatography
 - 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)

Recommended Books

1. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009).
 2. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry, 5th Ed.*, Pearson (2012)
 3. Vogel, A. I. *Elementary Practical Organic Chemistry, Part 2: Qualitative Organic Analysis*, CBS Publishers and Distributors.
 4. Bhattacharyya, R. C, *A Manual of Practical Chemistry*.
 5. Dutta, S, B. *Sc. Honours Practical Chemistry*, Bharati Book Stall.
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CHE-HC-2026: PHYSICAL CHEMISTRY II

(Credits: Theory-04, Practicals-02)

Course Objective: *In this course the chemical thermodynamics, chemical equilibrium, solutions and colligative properties will be taught to the students. Another unit of this course is systems of variable compositions.*

Learning Outcome: *In this course the students are expected to learn laws of thermodynamics, thermochemistry, thermodynamic functions, relations between thermodynamic properties, Gibbs Helmholtz equation, Maxwell relations etc. Moreover the students are expected to learn partial molar quantities, chemical equilibrium, solutions and colligative properties. After completion of this course, the students will be able to understand the chemical systems from thermodynamic point of view.*

Chemical Thermodynamics:

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 , relation between heat capacities, calculations of q , w , U and H for reversible, irreversible and free expansion of gases (ideal and van der Waals) under isothermal and adiabatic conditions. Law of equipartition of energy, degrees of freedom and molecular basis of heat capacities.

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: Concept of entropy; thermodynamic scale of temperature, statement of the second law of thermodynamics; molecular and statistical interpretation of entropy. Calculation of entropy change for reversible and irreversible processes.

Third Law: Statement of third law, concept of residual entropy, calculation of absolute entropy of molecules.

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

Systems of Variable Composition:

Partial molar quantities, dependence of thermodynamic parameters on composition; Gibbs-Duhem equation, chemical potential of ideal mixtures, change in thermodynamic functions in mixing of ideal gases.

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 K_p , K_c and K_x . Le Chatelier principle (quantitative treatment); equilibrium between ideal gases and a pure condensed phase.

Solutions and Colligative Properties:

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

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.

Recommended Books

1. Peter, A. & Paula, J. de. *Physical Chemistry 9th Ed.*, Oxford University Press (2011).
2. Castellan, G. W. *Physical Chemistry 4th Ed.*, Narosa (2004).
3. Engel, T. & Reid, P. *Physical Chemistry 3rd Ed.*, Prentice-Hall (2012).
4. McQuarrie, D. A. & Simon, J. D. *Molecular Thermodynamics* Viva Books Pvt. Ltd.: New Delhi (2004).
5. Assael, M. J.; Goodwin, A. R. H.; Stamatoudis, M.; Wakeham, W. A. & Will, S. *Commonly Asked Questions in Thermodynamics*. CRC Press: NY (2011).
6. Levine, I. N. *Physical Chemistry 6th Ed.*, Tata Mc Graw Hill (2010).
7. Metz, C.R. *2000 solved problems in chemistry*, Schaum Series (2006)
8. Puri, B. R.; Sharma, L. R.; Pathania, M. S. Principles of Physical Chemistry, Vishal Publishing Co.; 47th Ed. (2017)
9. Kapoor, K. L. A Textbook of Physical Chemistry (Volume 2) McGraw Hill Education; Sixth edition (2019)

CHE-HC-2026: LAB

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 basicity/proticity of a polyprotic acid by the thermochemical method in terms of the changes of temperatures observed in the graph of temperature versus time for different additions of a base. Also calculate the enthalpy of neutralization of the first step.
(f) Determination of enthalpy of hydration of copper sulphate.
(g) Study of the solubility of benzoic acid in water and determination of ΔH .

Any other experiment carried out in the class.

Recommended Books

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

Semester III

CHE-HC-3016: INORGANIC CHEMISTRY-II

(Credits: Theory-04, Practicals-02)

Course Objective: *This course starts with the basic principles of metallurgy so as to acquaint the students with the application of the redox chemistry they have learnt in the earlier course on inorganic chemistry. Concepts of protonic and non-protonic acids and bases are introduced for students to appreciate different types of chemical reactions. Periodic behavior of s and p block elements related to their electronic structure and their reactivity is included to acquaint students with the principles governing their reactivity. This course further intend to apprise students about the variety of compounds of the main group elements including oxides, hydrides, nitrides, interhalogens, noble gases and inorganic polymers. As part of the accompanying lab course, experiments involving iodo- and iodi-metric titrations are included for the students to explore other varieties of redox titration. Preparation of simple inorganic compounds is introduced to give hands-on experience of inorganic synthesis.*

Learning Outcome: *On successful completion of this course students would be able to apply theoretical principles of redox chemistry in the understanding of metallurgical processes. Students will be able to identify the variety of s and p block compounds and comprehend their preparation, structure, bonding, properties and uses. Experiments in this course will boost their quantitative estimation skills and introduce the students to preparative methods in inorganic chemistry.*

General Principles of Metallurgy

Chief modes of occurrence of metals based on standard electrode potentials. Ellingham diagrams for reduction of metal oxides using carbon and carbon monoxide as reducing agent. Electrolytic Reduction, Hydrometallurgy. Methods of purification of metals: Electrolytic Kroll process, Parting process, van Arkel-de Boer process and Mond's process, Zone refining.

Acids and Bases

Brönsted-Lowry concept of acid-base reactions, solvated proton, relative strength of acids, types of acid-base reactions, levelling solvents, Lewis acid-base concept, Classification of Lewis acids, Hard and Soft Acids and Bases (HSAB) Application of HSAB principle.

Chemistry of s and p Block Elements:

Inert pair 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.

Hydrides and their classification ionic, covalent and interstitial. Basic beryllium acetate and nitrate.

Study of the following compounds with emphasis on structure, bonding, preparation, properties and uses. Boric acid and borates, boron nitrogen compounds, boranes, carboranes and graphitic compounds, silanes, oxides and oxoacids of nitrogen, phosphorus and chlorine. Peroxo acids of sulphur, interhalogen compounds, polyhalide ions, pseudohalogens and basic properties of halogens.

Noble Gases:

Occurrence and uses, rationalization of inertness of noble gases, Clathrates; preparation and properties of XeF₂, XeF₄ and XeF₆; Nature of bonding in noble gas compounds (Valence bond treatment and MO treatment for XeF₂). Molecular shapes of noble gas compounds (VSEPR theory).

Inorganic Polymers:

Types of inorganic polymers, comparison with organic polymers, synthesis, structural aspects and applications of silicones and siloxanes. Silicates – clays and zeolites, polyphosphazenes, metal-organic framework compounds (MOFs).

Recommended Books:

1. Lee, J. D., Concise Inorganic Chemistry, 5th Ed., Oxford University Press, 2008.
2. Douglas, B.E. and Mc Daniel, D.H., Concepts and Models of Inorganic Chemistry, 3rd Ed. Wiley India, 2006.
3. Greenwood, N.N. & Earnshaw, A., Chemistry of the Elements, 2nd Ed., Elsevier India, 2010.
4. Cotton, F.A., Wilkinson, G. and Gaus, P. L., Basic Inorganic Chemistry, 3rd Ed., Wiley, 2007.
5. Cotton, F.A. & Wilkinson, G, Advanced Inorganic Chemistry. 6th Ed., Wiley-VCH, 2007.
6. Miessler, G. L. & Tarr, D. A., Inorganic Chemistry 4th Ed., Pearson, 2010.
7. Weller, M., Armstrong, F., Rourke, J. & Overton, T., Inorganic Chemistry 6th Ed. 2015.

CHE-HC-3016: LAB

60 Lectures

(A) Iodo / Iodimetric Titrations

- (i) Estimation of Cu(II) and K₂Cr₂O₇ using sodium thiosulphate solution (Iodimetrically).
- (ii) Estimation of (i) arsenite and (ii) antimony in tartar-emetic iodimetrically
- (iii) Estimation of available chlorine in bleaching powder iodometrically.

(B) Inorganic preparations

- (i) Cuprous Chloride, CuCl
- (ii) Preparation of manganese(III) phosphate, MnPO₄.H₂O
- (iii) Preparation of aluminium potassium sulphate KAl(SO₄)₂.12H₂O (Potash alum) or Chrome alum.

Recommended Books:

1. Mendham, J. et al.: Vogel's Text Book of Quantitative Chemical Analysis ; 6th Ed. Pearson Education, 2009.
2. Marr, G. and Rockett, R.W. *Practical Inorganic Chemistry*, Van Nostrand Reinhold. 1972.

CHE-HC-3026: ORGANIC CHEMISTRY-II

(Credits: Theory-04, Practicals-02)

Course Objectives: This course is intended to apprise students about different classes of organic compounds, including halogenated hydrocarbons, alcohols, phenols, epoxides, carbonyl compounds and carboxylic and sulfonic acids.

Students are expected to learn and differentiate between various organic functional groups; explain, analyze and design transformations between different functional groups.

Learning Outcome: Students will be able to describe and classify organic compounds in terms of their functional groups and reactivity.

Chemistry of Halogenated Hydrocarbons:

Alkyl halides: Methods of preparation, nucleophilic substitution reactions – S_N1, S_N2 and S_Ni mechanisms with stereochemical aspects and effect of solvent etc.; nucleophilic substitution vs. elimination.

Aryl halides: Preparation, including preparation from diazonium salts. nucleophilic aromatic substitution; S_NAr, Benzyne mechanism. Relative reactivity of alkyl, allyl/benzyl, vinyl and aryl halides towards nucleophilic substitution reactions.

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

(16 Lectures)

Alcohols, Phenols, Ethers and Epoxides:

Alcohols: preparation, properties and relative reactivity of 1°, 2°, 3° alcohols, Bouveault-Blanc Reduction; Preparation and properties of glycols: Oxidation by periodic acid and lead tetraacetate, Pinacol-Pinacolone rearrangement;

Phenols: Preparation and properties; Acidity and factors effecting it, Ring substitution reactions, Reimer-Tiemann and Kolbe's-Schmidt Reactions, Fries and Claisen rearrangements with mechanism;

Ethers and Epoxides: Preparation and reactions with acids. Reactions of epoxides with alcohols, ammonia derivatives and LiAlH₄

(16 Lectures)

Carbonyl Compounds:

Preparation, properties, structure and reactivity;

Nucleophilic additions, Nucleophilic addition-elimination reactions with ammonia derivatives with mechanism; Mechanisms of Aldol and Benzoin condensation, Knoevenagel condensation, Claisen-Schmidt, Perkin, Cannizzaro and Wittig reaction, Beckmann and Benzil-Benzilic acid rearrangements, haloform reaction and Baeyer Villiger oxidation, α-substitution reactions, oxidations and reductions (Clemmensen, Wolff-Kishner, LiAlH₄, NaBH₄, MPV, PDC and PGC);

Addition reactions of unsaturated carbonyl compounds: Michael addition.

Active methylene compounds: Keto-enol tautomerism. Preparation and synthetic applications of diethyl malonate and ethyl acetoacetate.

(14 Lectures)

Carboxylic Acids and their Derivatives:

Preparation, physical properties and reactions of monocarboxylic acids: Typical reactions of dicarboxylic acids, hydroxy acids and unsaturated acids: succinic/phthalic, lactic, malic, tartaric, citric, maleic and fumaric acids;

Preparation and reactions of acid chlorides, anhydrides, esters and amides; Comparative study of nucleophilic substitution at acyl group -Mechanism of acidic and alkaline hydrolysis of esters, Claisen condensation, Dieckmann and Reformatsky reactions, Hofmannbromamide

degradation and Curtius rearrangement.

(10 Lectures)

Sulphur containing compounds:

Preparation and reactions of thiols, thioethers and sulphonic acids.

(4 Lectures)

Recommended Books:

1. Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
3. Graham Solomons, T.W. *Organic Chemistry*, John Wiley & Sons, Inc.
4. Clayden, J., Greeves, N. & Warren, S. *Organic Chemistry*, Second edition, Oxford University Press, 2012.
5. Keeler, J., Wothers, P. *Chemical Structure and Reactivity – An Integrated approach*, Oxford University Press.
6. Smith, J. G. *Organic Chemistry*, Tata McGraw-Hill Publishing Company Limited.
7. Carey, F. A.; Sundberg, R. J. *Advanced Organic Chemistry: Reactions and Synthesis (Part B)*, Springer.

CHE-HC-3026: LAB

60 Lectures

1. Test of functional groups like alcohols, phenols, carbonyl and carboxylic acid group.
2. Organic preparations:
 - i. Acetylation of one of the following compounds: amines (aniline, *o*-, *m*-, *p*-toluidines *o*-, *m*-, *p*-anisidine) and phenols (β -naphthol, vanillin, salicylic acid) by any one method:
 - a. Using conventional method.
 - b. Using green approach
 - ii. Benzoylation of one of the following amines (aniline, *o*-, *m*-, *p*-toluidines and *o*-, *m*-, *p*-anisidine) and one of the following phenols (β -naphthol, resorcinol, *p*-cresol) by Schotten-Baumann reaction.
 - iii. Oxidation of ethanol/ isopropanol (Iodoform reaction).
 - iv. Bromination of any one of the following:
 - a. Acetanilide by conventional methods
 - b. Acetanilide using green approach (Bromate-bromide method)
 - v. Nitration of any one of the following:
 - a. Acetanilide/nitrobenzene by conventional method
 - b. Salicylic acid by green approach (using ceric ammonium nitrate).
 - vi. Selective reduction of *meta* dinitrobenzene to *m*-nitroaniline.
 - vii. Reduction of *p*-nitrobenzaldehyde by sodium borohydride.
 - viii. Hydrolysis of amides and esters.
 - ix. Semicarbazone of any one of the following compounds: acetone, ethyl methyl ketone, cyclohexanone, benzaldehyde.
 - x. *S*-Benzylisothiuronium salt of one each of water soluble and water insoluble acids (benzoic acid, oxalic acid, phenyl acetic acid and phthalic acid).
 - xi. Aldol condensation using either conventional or green method.
 - xii. Benzil-Benzilic acid rearrangement.

The above preparations should be done using 0.5-1g of the organic compound. The solid samples must be collected and may be used for recrystallization, melting point and TLC.

Recommended Books

1. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009)

2. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry, 5th Ed.*, Pearson (2012)
 3. Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis*, University Press (2000).
 4. Ahluwalia, V.K. & Dhingra, S. *Comprehensive Practical Organic Chemistry: Qualitative Analysis*, University Press (2000).
 5. Vogel, A. I. *Elementary Practical Organic Chemistry, Part 1: Small scale Preparations*, CBS Publishers and Distributors.
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CHE-HC-3036: PHYSICAL CHEMISTRY-III

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Course Objective: *The aim of this course is to teach students four important topics of physical chemistry- phase equilibria, chemical kinetics, surface chemistry and catalysis. Phase equilibria and chemical kinetics will be discussed in detail but surface chemistry and catalysis will be introduced to the students.*

Learning Outcome: *The students are expected to learn phase rule and its application in some specific systems. They will also learn rate laws of chemical transformation, experimental methods of rate law determination, steady state approximation etc. in chemical kinetics unit. After attending this course the students will be able to understand different types of surface adsorption processes and basics of catalysis including enzyme catalysis, acid base catalysis and particle size effect on catalysis.*

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.

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.

(28 Lectures)

Chemical Kinetics

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 (iv) chain reactions.

Temperature dependence of reaction rates; Arrhenius equation; activation energy. Collision theory of reaction rates, Lindemann mechanism, qualitative treatment of the theory of absolute reaction rates. Reaction mechanism- steady-state approximation and rate determining step approximation methods.

(18 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, acid-base catalysis.

(8 Lectures)

Surface chemistry:

Physical adsorption, chemisorption, adsorption isotherms, nature of adsorbed state.

(6 Lectures)

Recommended Books:

1. Peter Atkins & Julio De Paula, *Physical Chemistry 9th Ed.*, Oxford University Press(2010).
 2. Castellan, G. W. *Physical Chemistry*, 4th Ed., Narosa (2004).
 3. McQuarrie, D. A. & Simon, J. D., *Molecular Thermodynamics*, Viva Books Pvt. Ltd.:New Delhi (2004).
 4. Engel, T. & Reid, P. *Physical Chemistry 3rd Ed.*, Prentice-Hall (2012).
 5. Assael, M. J.; Goodwin, A. R. H.; Stamatoudis, M.; Wakeham, W. A. & Will, S. *Commonly Asked Questions in Thermodynamics*. CRC Press: NY (2011).
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 6. Zundhal, S.S. *Chemistry concepts and applications* Cengage India (2011).
 7. Ball, D. W. *Physical Chemistry* Cengage India (2012).
 8. Mortimer, R. G. *Physical Chemistry 3rd Ed.*, Elsevier: NOIDA, UP (2009).
 9. Levine, I. N. *Physical Chemistry 6th Ed.*, Tata McGraw-Hill (2011).
 10. Metz, C. R. *Physical Chemistry 2nd Ed.*, Tata McGraw-Hill (2009).
 11. Puri, B. R.; Sharma, L. R.; Pathania, M. S. Principles of Physical Chemistry, Vishal Publishing Co.; 47th Ed. (2017)
 12. Kapoor, K. L. A Textbook of Physical Chemistry (Volume 5) McGraw Hill Education; 5th edition (2017)
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CHE-HC-3036: LAB

60 Lectures

- I. Determination of critical solution temperature and composition of the phenol-water system and to study the effect of impurities on it.
- II. Phase equilibria: Construction of the phase diagram using cooling curves or ignition tube method:a. simple eutectic and b. congruently melting systems.
- III. Distribution of acetic/ benzoic acid between water and cyclohexane.
- IV. Study the equilibrium of at least one of the following reactions by the distribution method:
 - (i) $I_2(aq) + I \rightarrow I_3(aq)_{2+}$
 - (ii) $Cu_{2+}(aq) + nNH_3 \rightarrow Cu(NH_3)_n$
- V. Study the kinetics of the following reactions.
 1. Initial rate method: Iodide-persulphate reaction
 2. Integrated rate method:
 - a. Acid hydrolysis of methyl acetate with hydrochloric acid.
 - b. Saponification of ethyl acetate.
 3. Compare the strengths of HCl and H₂SO₄ by studying kinetics of hydrolysis of methyl acetate.
- VI. Adsorption
 - I. Verify the Freundlich and Langmuir isotherms for adsorption of acetic acid on activated charcoal.

Recommended Books:

1. Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).

2. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8th Ed.*; McGraw-Hill: New York (2003).
3. Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry 3rd Ed.*; W.H. Freeman & Co.: New York (2003).
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Semester IV

CHE-HC-4016: INORGANIC CHEMISTRY-III

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Course Objective: This course introduces students to coordination chemistry. Various aspects like nomenclature, structure, bonding, variety and reactivity of the coordination compounds are included for the students to appreciate.

Bioinorganic chemistry is included in this course to acquaint students on the useful and harmful aspects of metals in biological systems.

Through the accompanying lab course, experiments related to gravimetric analysis, synthesis of coordination compounds and separation of metal ions using chromatography is included.

This will broaden the experimental skills of the students where students will learn about various aspects of experiment design depending upon the requirements like synthesis, estimation or separation.

Learning Outcome: On successful completion, students will be able name coordination compounds according to IUPAC, explain bonding in this class of compounds, understand their various properties in terms of CFSE and predict reactivity. Students will be able to appreciate the general trends in the properties of transition elements in the periodic table and identify differences among the rows.

Through the experiments students not only will be able to prepare, estimate or separate metal complexes/compounds but also will be able to design experiments independently which they should be able to apply if and when required.

Coordination Chemistry:

Coordination compounds, types of ligands, Werner's theory, IUPAC nomenclature and 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 $10 Dq$ (Δ_o), CFSE in weak and strong fields, pairing energies, factors affecting the magnitude of $10 Dq$ (Δ_o , Δ_t). Octahedral vs. tetrahedral coordination, tetragonal distortions from octahedral geometry Jahn-Teller theorem, square planar geometry. Qualitative aspects of ligand field and MO Theory.

Chelate effect, polynuclear complexes, labile and inert complexes. **(26 Lectures)**

Transition Elements:

General group trends with special reference to electronic configuration, colour, variable valency, magnetic and catalytic properties, ability to form complexes. Stability of various oxidation states and e.m.f. (Latimer & Frost diagrams). Difference between the first, second and third transition series.

Chemistry of Ti, V, Cr Mn, Fe and Co (Chemistry of first -row transition elements) in various oxidation states as halides, oxides, hydroxides. **(18 Lectures)**

Lanthanoids and Actinoids:

Electronic configuration, oxidation states, colour, spectral and magnetic properties, lanthanide contraction, separation of lanthanides (ion-exchange method only). **(6 Lectures)**

Bioinorganic Chemistry:

Metal ions present in biological systems, classification of elements according to their action in biological system. Geochemical effect on the distribution of metals. Sodium / K-pump, carbonic anhydrase and carboxypeptidase. Excess and deficiency of some trace metals. Toxicity of metal ions (Hg, Pb, Cd and As), reasons for toxicity, Use of chelating agents in medicine. Iron and its application in bio-systems, Haemoglobin; Storage and transfer of iron. (10 Lectures)

Recommended Books:

1. Cotton, F.A., Wilkinson, G. and Gaus, P. L., Basic Inorganic Chemistry, 3rd Ed., Wiley, 2007.
 2. Huheey, J. E., Keiter, E. A., Keiter, R. L., Medhi, O. K., Inorganic Chemistry: Principles of Structure and Reactivity, 4th Ed., Pearson Education India, 2006.
 3. Lippard, S.J. & Berg, J.M. Principles of Bioinorganic Chemistry, Panima Publishing Company, 1994.
 4. Cotton, F.A. & Wilkinson, G, Advanced Inorganic Chemistry. 6th Ed., Wiley-VCH, 2007.
 5. Basolo, F, and Pearson, R.C., Mechanisms of Inorganic Chemistry, John Wiley & Sons, NY, 1967.
 6. Greenwood, N.N. & Earnshaw, A., Chemistry of the Elements, 2nd Ed., Elsevier India, 2010.
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CHE-HC-4016: LAB

60 Lectures

Gravimetric Analysis:

- i. Estimation of nickel(II) using dimethylglyoxime (DMG).
- ii. Estimation of copper as CuSCN
- iii. Estimation of iron as Fe₂O₃ by precipitating iron as Fe(OH)₃.
- iv. Estimation of Al (III) by precipitating with oxine and weighing as Al(oxine)₃ (aluminiumoxinate).

Inorganic Preparations:

- i. Tetraamminecopper(II) sulphate, [Cu(NH₃)₄]SO₄.H₂O
- ii. *Cis* and *trans* K[Cr(C₂O₄)₂.(H₂O)₂] Potassium dioxalatodiaquachromate (III)
- iii. Tetraamminecarbonatocobalt (III) ion
- iv. Potassium tris(oxalato)ferrate(III)

Chromatography of metal ions

Principles involved in chromatographic separations. Paper chromatographic separation of following metal ions:

- i. Ni(II) and Co(II)
- ii. Fe(III) and Al(III)

Recommended Book:

1. Mendham, J. et al.: Vogel's Textbook of Quantitative Chemical Analysis ; 6th Ed. Pearson Education, 2009.
 2. Marr, G. and Rickett, R.W. *Practical Inorganic Chemistry*, Van Nostrand Reinhold. 1972.
 3. *Inorganic Syntheses*, Vol. 1-10.
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CHE-HC-4026: ORGANIC CHEMISTRY-III **(Credits: Theory-04, Practicals-02)**

Course Objectives: The course intrudes students to different classes of N-based compounds, including alkaloids and terpenoids and their potential application.

Students are expected to learn about different classes of N-based compounds; their structures, synthesis and reactivity.

Learning Outcome: Students shall demonstrate the ability to identify and classify different types of N-based derivatives, alkaloids and hetrocyclic compounds/explain their structure mechanism and reactivity/critically examine their synthesis and reactions mechanism.

Nitrogen Containing Functional Groups

Preparation and important reactions of nitro and compounds, nitriles and isonitriles

Amines: Effect of substituent and solvent on basicity; Preparation and properties: 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.

Diazonium Salts: Preparation and their synthetic applications. **(18 Lectures)**

Polynuclear Hydrocarbons

Reactions of naphthalene phenanthrene and anthracene Structure, Preparation and structure elucidation and important derivatives of naphthalene and anthracene; Polynuclear hydrocarbons. **(8 Lectures)**

Heterocyclic Compounds

Classification and nomenclature, Structure, aromaticity in 5-numbered and 6-membered rings containing 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. Indole: Fischer indole synthesis and Madelung synthesis). Quinoline and isoquinoline: Skraup synthesis, Friedlander's synthesis, Knorr quinoline synthesis, Doebner- Miller synthesis, Bischler-Napieralski reaction, Pictet-Spengler reaction, Pomeranz-Fritsch reaction **(22 Lectures)**

Alkaloids

Natural occurrence, General structural features, Isolation and their physiological action

Hoffmann's exhaustive methylation, Emde's modification, Structure elucidation and synthesis of Nicotine. Medicinal importance of Nicotine, Hygrine, Quinine, Morphine, Cocaine, and Reserpine. **(6 Lectures)**

Terpenes

Occurrence, classification, isoprene rule; Elucidation of structure and synthesis of Citral, Neral and α -terpineol. **(6 Lectures)**

Recommended Books:

1. Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
3. Finar, I. L. *Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
4. Graham Solomons, T.W. *Organic Chemistry*, John Wiley & Sons, Inc.
5. Kalsi, P. S. *Textbook of Organic Chemistry 1st Ed.*, New Age International (P) Ltd. Pub.

6. Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; *Organic Chemistry*, Oxford University Press.
 7. Singh, J.; Ali, S.M. & Singh, J. *Natural Product Chemistry*, Prajati Parakashan (2010). (2010).
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CHE-HC-4026: LAB

60 Lectures

1. Detection N, S, halogens in organic compounds.
2. Functional group test for nitro, amine and amide groups.
3. Qualitative analysis of unknown organic compounds containing simple functional groups (alcohols, carboxylic acids, phenols and carbonyl compounds)

Recommended Books

1. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009)
 2. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry, 5th Ed.*, Pearson (2012)
 3. Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis*, University Press (2000).
 4. Ahluwalia, V.K. & Dhingra, S. *Comprehensive Practical Organic Chemistry: Qualitative Analysis*, University Press (2000).
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CHE-HC-4036: PHYSICAL CHEMISTRY-IV

(Credits: Theory-04, Practicals-02)

Course Objective: The aim of this course is to introduce students with primarily two areas of physical chemistry- electrochemistry and electrical and magnetic properties of atoms and molecules. It contains three units- conductance, electrochemistry and electrical & magnetic properties of atoms and molecules.

Learning Outcome: In this course the students will learn theories of conductance and electrochemistry. Students will also understand some very important topics such as solubility and solubility products, ionic products of water, conductometric titrations etc. The students are also expected to understand the various parts of electrochemical cells along with Faraday's Laws of electrolysis. The students will also gain basic theoretical idea of electrical & magnetic properties of atoms and molecules.

Conductance

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. Debye-Hückel-Onsager equation, Wien effect, Debye-Falkenhagen effect, Walden's rules. 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.

Electrochemistry

Quantitative aspects of Faraday's laws of electrolysis, rules of oxidation/reduction of ions based on half-cell potentials.

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 $\text{SbO/Sb}_2\text{O}_3$ 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). Applications of electrolysis in metallurgy and industry.

Electrical & Magnetic Properties of Atoms and Molecules

Basic ideas of electrostatics, Electrostatics of dielectric media, Clausius-Mosotti equation, Lorenz-Laurentz equation, Dipole moment and molecular polarizabilities and their measurements. Diamagnetism, paramagnetism, magnetic susceptibility and its measurement, molecular interpretation.

Recommended Books:

1. Atkins, P.W & Paula, J.D. *Physical Chemistry*, 9th Ed., Oxford University Press (2011).
2. Castellan, G. W. *Physical Chemistry 4th Ed.*, Narosa (2004).
3. Mortimer, R. G. *Physical Chemistry 3rd Ed.*, Elsevier: NOIDA, UP (2009).
4. Barrow, G. M., *Physical Chemistry 5th Ed.*, Tata McGraw Hill: New Delhi (2006).
5. Engel, T. & Reid, P. *Physical Chemistry 3rd Ed.*, Prentice-Hall (2012).
6. Rogers, D. W. *Concise Physical Chemistry* Wiley (2010).
7. Silbey, R. J.; Alberty, R. A. & Bawendi, M. G. *Physical Chemistry 4th Ed.*, John Wiley & Sons, Inc. (2005).
8. Puri, B. R.; Sharma, L. R.; Pathania, M. S. Principles of Physical Chemistry, Vishal Publishing Co.; 47th Ed. (2017)
9. Kapoor, K. L. A Textbook of Physical Chemistry (Volume 1) McGraw Hill Education; Sixth edition (2019)

CHE-HC-4036: LAB

60 Lectures

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:
 - i. Strong acid vs. strong base
 - ii. Weak acid vs. strong base
 - iii. Mixture of strong acid and weak acid vs. strong base
 - iv. Strong acid vs. weak base

Potentiometry

I Perform the following potentiometric titrations:

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- 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

Recommended Books:

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

CHE-HC-5016: ORGANIC CHEMISTRY-IV**(Credits: Theory-04, Practicals-02)**

Course Objectives: This course introduces students to nucleic acids, amino acids and pharmaceutical compounds.

Students will be familiarized with the importance of nucleic acids, amino acids and develop basic understanding of enzymes, bioenergetics and pharmaceutical compounds.

Learning Outcome: Students will be able to explain/describe the important features of nucleic acids, amino acids and enzymes and develop their ability to examine their properties and applications.

Nucleic Acids

Components of nucleic acids; Nucleosides and nucleotides;

Synthesis and reactions of: Adenine, Guanine, Cytosine, Uracil and Thymine;

Polynucleotides: DNA and RNA

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

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).

Lipids

Introduction to oils and fats; common fatty acids present in oils and fats, Hydrogenation of fats and oils, saponification value, acid value, iodine number, rancidity.

Concept of Energy in Biosystems

Cells obtain energy by the oxidation of foodstuff (organic molecules).

Introduction to metabolism (catabolism, anabolism).

ATP: The universal currency of cellular energy, ATP hydrolysis and free energy change.

Agents for transfer of electrons in biological redox systems: NAD^+ , FAD.

Conversion of food to energy: Outline of catabolic pathways of carbohydrate- glycolysis,

fermentation, Krebs cycle.

Overview of catabolic pathways of fat and protein.

Interrelationship in the metabolic pathways of protein, fat and carbohydrate.

Calorific value of food, standard calorie content of food types.

Pharmaceutical Compounds: Structure and Importance

Classification, structure and therapeutic uses of antipyretics: Paracetamol (with synthesis), Analgesics: Ibuprofen (with synthesis), Antimalarials: Chloroquine (with synthesis). An elementary treatment of Antibiotics and detailed study of chloramphenicol, Medicinal values of curcumin (turmeric), azadirachtin (neem), vitamin C and antacid (ranitidine).

Recommended Books:

1. Berg, J.M., Tymoczko, J.L. and Stryer, L. (2006) Biochemistry. VIth Edition. W.H. Freeman and Co.
2. Nelson, D.L., Cox, M.M. and Lehninger, A.L. (2009) Principles of Biochemistry. IV Edition. W.H. Freeman and Co.
3. Murray, R.K., Granner, D.K., Mayes, P.A. and Rodwell, V.W. (2009) Harper's Illustrated Biochemistry. XXVIII edition. Lange Medical Books/ McGraw-Hill.

CHE-HC-5016: LAB

1. Estimation of glycine by Sorenson's formalin method.
2. Study of the titration curve of glycine.
3. Estimation of proteins by Lowry's method.
4. Study of the action of salivary amylase on starch at optimum conditions.
5. Effect of temperature on the action of salivary amylase.
6. Saponification value of an oil or a fat.
7. Determination of Iodine number of an oil/ fat.
8. Isolation and characterization of DNA from onion/ cauliflower/peas.

Recommended Books:

1. Arthur, I. V. *Quantitative Organic Analysis*, Pearson.
2. Plummer, D. T. *An Introduction to Practical Biochemistry*, 3rd Edition, McGraw Hill.

CHE-HC-5026: PHYSICAL CHEMISTRY V

(Credits: Theory-04, Practicals-02)

Course Objective: *The aim of this course is to introduce the students with three important areas- quantum chemistry, molecular spectroscopy and photochemistry. In quantum chemistry unit the students will be taught the postulates of quantum mechanics and the application of quantum mechanical ideas in some simple systems such as particle in a box, rigid rotor, simple harmonic oscillator etc. In spectroscopy unit, rotational, vibrational, Raman, electronic, spin resonance, and electronic spectroscopy will be introduced.*

Learning Outcome: *After completion of this course the students are expected to understand the application of quantum mechanics in some simple chemical systems such as hydrogen atom or hydrogen like ions. The students will also learn chemical bonding in some simple molecular systems. They will be able to understand the basics of various kinds of spectroscopic techniques and photochemistry.*

Quantum Chemistry:

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 levels, zero-point energy Extension to two and three dimensional boxes, separation of variables, degeneracy.

Qualitative treatment of simple harmonic oscillator model of vibrational motion: Setting up of Schrödinger equation and discussion of solution and wavefunctions. Vibrational energy of diatomic molecules and zero-point energy.

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

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

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). Need for approximation methods. Statement of variation theorem and application to simple systems (particle-in-a-box, harmonic oscillator, hydrogen atom).

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 and heteronuclear diatomic molecules (HF, LiH). Localised and non-localised molecular orbitals treatment of triatomic (BeH_2 , H_2O) molecules. Qualitative MO theory and its application to AH_2 type molecules.

Molecular Spectroscopy:

Interaction of electromagnetic radiation with molecules and various types of spectra; Born-Oppenheimer approximation.

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.

Electronic spectroscopy: Franck-Condon principle, electronic transitions, singlet and triplet states, fluorescence and phosphorescence, dissociation and predissociation, calculation of electronic transitions of polyenes using free electron model.

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. Role of photochemical reactions in biochemical processes, photostationary states, chemiluminescence.

Recommended Books:

1. Banwell, C. N. & McCash, E. M. Fundamentals of Molecular Spectroscopy 4th Ed. Tata McGraw-Hill: New Delhi (2006).
2. Chandra, A. K. Introductory Quantum Chemistry Tata McGraw-Hill (2001).
3. House, J. E. Fundamentals of Quantum Chemistry 2nd Ed. Elsevier: USA (2004).

4. Lowe, J. P. & Peterson, K. Quantum Chemistry, Academic Press (2005).
 5. Kakkar, R. Atomic & Molecular Spectroscopy, Cambridge University Press (2015).
 6. Kapoor, K. L. A Textbook of Physical Chemistry (Volume 4) McGraw Hill Education; 5th edition (2017)
 7. Sen, B. K. Quantum Chemistry- Including Spectroscopy, Kalyani Publishers; 4th edition (2011)
 8. McQuarrie, D. A. Quantum Chemistry, Viva Books (2016)
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CHE-HC-5026: LAB

UV/Visible spectroscopy

- I. Study the 200-500 nm absorbance spectra of KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$ (in 0.1 M H_2SO_4) and determine the λ_{max} values. Calculate the energies of the two transitions in different units (J molecule^{-1} , kJ mol^{-1} , cm^{-1} , eV).
- II. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of $\text{K}_2\text{Cr}_2\text{O}_7$.
- III. Record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde, 2-propanol, acetic acid) in water. Comment on the effect of structure on the UV spectra of organic compounds.

Colourimetry

- I. Verify Lambert-Beer's law and determine the concentration of $\text{CuSO}_4/\text{KMnO}_4/\text{K}_2\text{Cr}_2\text{O}_7$ in a solution of unknown concentration
- II. Determine the concentrations of KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$ in a mixture.
- III. Study the kinetics of iodination of propanone in acidic medium.
- IV. Determine the amount of iron present in a sample using 1,10-phenanthroline.
- V. Determine the dissociation constant of an indicator (phenolphthalein).
- VI. Study the kinetics of interaction of crystal violet/ phenolphthalein with sodium hydroxide.
- VII. Analysis of the given vibration-rotation spectrum of $\text{HCl}(\text{g})$

Recommended Books

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

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Semester VI

CHE-HC-6016: INORGANIC CHEMISTRY-IV

(Credits: Theory-04, Practicals-02)

Course Objective: The unit on reaction mechanism is included for the students to get acquainted with the kinetic and thermodynamic factors governing the reaction path and stability of inorganic compounds.

Organometallic compounds are introduced so as to apprise students about the importance of metal carbon bond to form complexes and their application as catalysts. Students are expected to learn factors leading to stability of organometallic compounds, their synthesis, reactivity and uses.

Qualitative inorganic analysis is included to give students an idea and hands on experience of application of inorganic chemistry. Students should learn how differential reactivity under

different conditions of pH can be used to identify variety of ions in a complex mixture. Experiments related to synthesis and characterization of coordination compounds are included to supplement their theoretical knowledge.

Learning Outcome: *By studying this course the students will be expected to learn about how ligand substitution and redox reactions take place in coordination complexes.*

Students will also learn about organometallic compounds, comprehend their bonding, stability, reactivity and uses. They will be familiar with the variety of catalysts based on transition metals and their application in industry.

On successful completion, students in general will be able to appreciate the use of concepts like solubility product, common ion effect, pH etc. in analysis of ions and how a clever design of reactions, it is possible to identify the components in a mixture.

With the experiments related to coordination compound synthesis, calculation of $10Dq$, controlling factors etc. will make the students appreciate the concepts of theory in experiments.

Mechanism of Inorganic Reactions

Introduction to inorganic reaction mechanisms. Substitution reactions in square planar complexes, Trans-effect, theories of trans effect, Mechanism of nucleophilic substitution in square planar complexes, Thermodynamic and Kinetic stability, Kinetics of octahedral substitution, Ligand field effects and reaction rates, Mechanism of substitution in octahedral complexes. Electron transfer reactions.

Organometallic Compounds

Definition and classification of organometallic compounds on the basis of bond type.

Concept of hapticity of organic ligands.

Metal carbonyls: 18 electron rule, 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.

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.

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

Transition Metals in Catalysis

Study of the following industrial processes and their mechanism:

1. Alkene hydrogenation (Wilkinson's Catalyst)
2. Hydroformylation (Co catalysts)
3. Wacker Process
4. Synthetic gasoline (Fischer Tropsch reaction)
5. Synthesis gas by metal carbonyl complexes

Theoretical Principles in Qualitative Inorganic Analysis (H₂S Scheme)

Basic principles involved in analysis of cations and anions and solubility products, common ion effect. Principles involved in separation of cations into groups and choice of group reagents. Interfering anions (fluoride, borate, oxalate and phosphate) and need to remove them after Group II.

Recommended Books:

1. Vogel, A.I. *Qualitative Inorganic Analysis*, Longman, 1972.
2. Svehla, G. & Sivasankar, B., *Vogel's Qualitative Inorganic Analysis*, 7th Ed., Prentice Hall, 2012.
3. Cotton, F.A., Wilkinson, G. and Gaus, P. L., *Basic Inorganic Chemistry*, 3rd Ed., Wiley, 2007.
4. Cotton, F.A. & Wilkinson, G, *Advanced Inorganic Chemistry*. 6th Ed., Wiley-VCH, 2007.
5. Huheey, J. E., Keiter, E. A., Keiter, R. L., Medhi, O. K., *Inorganic Chemistry: Principles of Structure and Reactivity*, 4th Ed., Pearson Education India, 2006.
6. Sharpe, A.G. *Inorganic Chemistry*, 4th Indian Reprint (Pearson Education) 2005
7. Douglas, B.E. and Mc Daniel, D.H., *Concepts and Models of Inorganic Chemistry*, 3rd Ed. Wiley India, 2006.
8. Greenwood, N.N. & Earnshaw, A., *Chemistry of the Elements*, 2nd Ed., Elsevier India, 2010.
9. Lee, J. D., *Concise Inorganic Chemistry*, 5th Ed., Oxford University Press, 2008.
10. Powell, P. *Principles of Organometallic Chemistry*, Chapman and Hall, 1988.
11. Shriver, D.D. & Atkins, P., *Inorganic Chemistry 2nd Ed.*, Oxford University Press, 1994.
12. Basolo, F. & Person, R. *Mechanisms of Inorganic Reactions: Study of Metal Complexes in Solution* 2nd Ed., John Wiley & Sons Inc; NY.
13. Purcell, K.F. & Kotz, J.C., *Inorganic Chemistry*, W.B. Saunders Co. 1977
14. Miessler, G. L. & Tarr, D. A., *Inorganic Chemistry* 4th Ed., Pearson, 2010.
15. Crabtree, Robert H. *The Organometallic Chemistry of the Transition Metals*. j New York, NY: John Wiley, 2000.
16. Spessard, Gary O., & Gary L. Miessler. *Organometallic Chemistry*. Upper Saddle River, NJ: Prentice-Hall, 1996.

CHE-HC-6016: LAB

60 Lectures

• Qualitative semimicro analysis of mixtures containing 3 anions and 3 cations. Emphasis should be given to the understanding of the chemistry of different reactions. The following radicals are suggested: CO_3

2^- , NO_2

$^-$, S_2^- , SO_3

2^- , S_2O_3

2^- , CH_3COO^- , F^- , Cl^- , Br^- , I^- , NO_3

$^-$,

BO_3

3^- , C_2O_4

2^- , PO_4

3^- , NH_4

$+$, K^+ , Pb^{2+} , Cu^{2+} , Cd^{2+} , Bi^{3+} , Sn^{2+} , Sb^{3+} , Fe^{3+} , Al^{3+} , Cr^{3+} , Zn^{2+} ,

Mn^{2+} , Co^{2+} , Ni^{2+} , Ba^{2+} , Sr^{2+} , Ca^{2+} , Mg^{2+}

• 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 e.g. CO_3

2^- and SO_3

2^- , NO_2

and

NO_3

-, Cl- and Br-, Cl- and I-, Br- and I-, NO₃
- and Br-, NO₃
- and I-

- Spot tests should be done whenever possible.
- Synthesis of ammine complexes of Ni(II) and their ligand exchange reactions involving bidentate ligands like acetylacetonate, dimethylglyoxime, glycine, etc.
- Preparation of acetylacetonate complexes of Cu²⁺/Fe³⁺.
- Controlled synthesis of two copper oxalate hydrate complexes: kinetic vs. thermodynamic factors.
- Determination of ϵ_{max} value from UV-visible spectra of complexes.
- Measurement of 10 Dq by spectrophotometric method, verification of spectrochemical series.

Recommended Books

1. Vogel's *Qualitative Inorganic Analysis*, Revised by G. Svehla.
 2. Marr, G. and Rockett, R.W. *Practical Inorganic Chemistry*, Van Nostrand Reinhold. 1972.
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CHE-HC-6026: ORGANIC CHEMISTRY-V (Credits: Theory-04, Practicals-02)

Course Objectives: This is a basic course in organic spectroscopy and provides introduction to carbohydrate chemistry, dyes and polymers.

Students are expected to learn about the different spectroscopic techniques and their applications in organic chemistry. Students shall be apprised with carbohydrate chemistry, dyes and polymers and their structure, reactivity and chemical properties.

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Learning Outcome: Students will be able to explain/describe basic principles of different spectroscopic techniques and their importance in chemical/organic analysis. Students shall be able to classify/identify/critically examine carbohydrates, polymers and dye materials.

Spectroscopy

Introduction to absorption and emission spectroscopy.

UV Spectroscopy: Types of electronic transitions, λ_{max} , Chromophores and Auxochromes, Bathochromic and Hypsochromic shifts, Intensity of absorption; Application of Woodward Rules for calculation of λ_{max} for the following systems: α,β unsaturated aldehydes, ketones, carboxylic acids and esters; Conjugated dienes: alicyclic, homoannular and heteroannular; Extended conjugated systems (aldehydes, ketones and dienes); 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; application in functional group analysis.

NMR Spectroscopy: Basic principles of Proton Magnetic Resonance, chemical shift and factors influencing it; Spin – Spin coupling and coupling constant; Anisotropic effects in alkene, alkyne, aldehydes and aromatics, Interpretation of NMR spectra of simple compounds. Electron Spin Resonance (ESR) spectroscopy: Its principle, hyperfine structure, ESR of simple radicals.

Applications of IR, UV and NMR for identification of simple organic and inorganic molecules.

Carbohydrates

Occurrence, classification and their biological importance.

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; Killiani-Fischer synthesis and Ruff degradation;

Disaccharides – Structure elucidation of maltose, lactose and sucrose.

Polysaccharides – Elementary treatment of starch, cellulose and glycogen.

Dyes

Classification, Colour and constitution; Mordant and Vat Dyes; Synthesis and applications of: Azo dyes – Methyl Orange and Congo Red (mechanism of Diazo Coupling); Triphenyl Methane Dyes – Malachite Green, Rosaniline and Crystal Violet; Phthalein Dyes – Phenolphthalein and Fluorescein; Natural dyes synthesis of Alizarin and Indigotin; Edible Dyes with examples.

Polymers

Introduction and classification.

Number average molecular weight, Weight average molecular weight, Degree of polymerization, Polydispersity Index.

Polymerisation reactions -Addition and condensation -Mechanism of cationic, anionic and free radical addition polymerization; Preparation and applications of plastics – thermosetting (phenol-formaldehyde, Polyurethanes) and thermosoftening (PVC, polythene);

Fabrics – natural and synthetic (acrylic, polyamido, polyester); Rubbers – natural and synthetic: Buna-S, Chloroprene and Neoprene; Vulcanization; Polymer additives;

Introduction to liquid crystal polymers; Biodegradable and conducting polymers with examples.

Recommended Books:

1. Banwell, C. N. & Mc.Cash, E. M. *Fundamentals of Molecular Spectroscopy*, 4th Edition, McGraw Hill.
2. Pavia, Lampman, Kriz & Vyvyan, *Introduction to Spectroscopy*, 5th Edition, CENGAGE Learning.
3. Silverstein, R. M.; Webster, F. X.; Kiemle, D. J. & Bryce, D. L. *Spectrometric Identification of Organic Compounds*, 8th Edition, Wiley.
4. Kemp, W. *Organic Spectroscopy*, Palgrave.
5. Kalsi, P. S. *Textbook of Organic Chemistry 1st Ed.*, New Age International (P) Ltd. Pub.
6. Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
7. Billmeyer, F. W. *Textbook of Polymer Science*, John Wiley & Sons, Inc.
8. Gowariker, V. R.; Viswanathan, N. V. & Sreedhar, J. *Polymer Science*, New Age International (P) Ltd. Pub.
9. Finar, I. L. *Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
10. Graham Solomons, T.W. *Organic Chemistry*, John Wiley & Sons, Inc.
11. Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; *Organic Chemistry*, Oxford University Press.
12. Singh, J.; Ali, S.M. & Singh, J. *Natural Product Chemistry*, Prajati Prakashan (2010).

CHE-HC-6026: LAB

1. Extraction of caffeine from tea leaves.
2. Preparation of sodium polyacrylate.
3. Preparation of urea formaldehyde.
4. Analysis of Carbohydrate: aldoses and ketoses, reducing and non-reducing sugars

5. Qualitative analysis of unknown organic compounds containing monofunctional groups (carbohydrates, aryl halides, aromatic hydrocarbons, nitro compounds, amines and amides) and simple bifunctional groups, for e.g. salicylic acid, cinnamic acid, nitrophenols etc.
6. Identification of simple organic compounds by IR spectroscopy and NMR spectroscopy (Spectra to be provided).
7. Preparation of methyl orange.

Recommended Books:

1. Vogel, A.I. *Quantitative Organic Analysis*, Part 3, Pearson (2012).
2. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009)
3. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry*, 5th Ed., Pearson (2012)
4. Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis*, University Press (2000).
5. Ahluwalia, V.K. & Dhingra, S. *Comprehensive Practical Organic Chemistry: Qualitative Analysis*, University Press (2000).

CHEMISTRY-Discipline Specific Electives (DSE)

CHE-HE-5014: APPLICATIONS OF COMPUTERS IN CHEMISTRY (Credits: Theory-04, Practicals-02)

Course Objective: This course intends to make learners familiar with basics of computer language, computer programming, handling of experimental data, curve fitting etc to analyze experimental results. This basic knowledge will help the students to perform and interpret results of various chemistry practicals.

Learning Outcome: After the completion of this course it will help the student to interpret laboratory data, curve fitting of experimental work, also perform quantum mechanical calculations for various molecular models.

Basics:

Constants, variables, bits, bytes, binary and ASCII formats, arithmetic expressions, hierarchy of operations, inbuilt functions. Elements of the BASIC language. 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.

Numerical methods:

Roots of equations: Numerical methods for roots of equations: Quadratic formula, iterative method, Newton-Raphson method, Binary bisection and Regula-Falsi.

Differential calculus: Numerical differentiation.

Integral calculus: Numerical integration (Trapezoidal and Simpson's rule), probability distributions and mean values.

Simultaneous equations: Matrix manipulation: addition, multiplication. Gauss-Siedal method.

Interpolation, extrapolation and curve fitting: Handling of experimental data.

Conceptual background of molecular modelling: Potential energy surfaces. Elementary ideas of molecular mechanics and practical MO methods.

Recommended Books:

1. Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007) Chapters 3-5.
2. Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis*, Cambridge Univ. Press (2001) 487 pages.

3. Noggle, J. H. *Physical chemistry on a Microcomputer*. Little Brown & Co. (1985).
 4. Venit, S.M. *Programming in BASIC: Problem solving with structure and style*. Jaico Publishing House: Delhi (1996).
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CHE-HE-5014: Lab

Computer programs based on numerical methods for

1. Roots of equations: (e.g. volume of van der Waals gas and comparison with ideal gas, pH of a weak acid).
2. Numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations).
3. Numerical integration (e.g. entropy/ enthalpy change from heat capacity data), probability distributions (gas kinetic theory) and mean values.
4. Matrix operations. Application of Gauss-Siedel method in colourimetry.
5. Simple exercises using molecular visualization software.

Recommended Books:

1. McQuarrie, D. A. *Mathematics for Physical Chemistry* University Science Books (2008).
 2. Mortimer, R. *Mathematics for Physical Chemistry*. 3rd Ed. Elsevier (2005).
 3. Steiner, E. *The Chemical Maths Book* Oxford University Press (1996).
 4. Yates, P. *Chemical Calculations*. 2nd Ed. CRC Press (2007).
 5. Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007) Chapters 3-5.
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 6. Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis*, Cambridge Univ. Press (2001) 487 pages.
 7. Noggle, J. H. *Physical Chemistry on a Microcomputer*. Little Brown & Co. (1985).
 8. Venit, S.M. *Programming in BASIC: Problem solving with structure and style*. Jaico Publishing House: Delhi (1996).
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CHE-HE-5024: ANALYTICAL METHODS IN CHEMISTRY

(Credits: Theory-04, Practicals-02)

Course Objective: *This is an elective course designed to complement the needs of students who wish to learn more about the qualitative/quantitative characterization and separation techniques. The content of this course aims to cover some of the widely used instrumental techniques for characterization of samples. Experiments included aim at giving students hands on experience using different instrumental techniques and chemical analysis.*

Learning outcome: *On successful completion students will be have theoretical understanding about choice of various analytical techniques used for qualitative and quantitative characterization of samples. At the same time through the experiments students will gain hands on experience of the discussed techniques. This will enable students to take judicious decisions while analyzing different samples.*

Qualitative and quantitative aspects of analysis:

Sampling, evaluation of analytical data, errors, accuracy and precision, methods of their expression, normal law of distribution if indeterminate errors, statistical test of data; F, Q and t test, rejection of data, and confidence intervals.

Optical methods of analysis:

Origin of spectra, interaction of radiation with matter, fundamental laws of spectroscopy and

selection rules, validity of Beer-Lambert's law.

UV-Visible Spectrometry: Basic principles of instrumentation (choice of source, monochromator and detector) for single and double beam instrument;

Basic principles of quantitative analysis: estimation of metal ions from aqueous solution, geometrical isomers, keto-enol tautomers. Determination of metal complex composition using Job's method of continuous variation and mole ratio method.

Infrared Spectroscopy: Basic principles of instrumentation (choice of source, monochromator & detector) for continuous wave and Fourier transform spectrometers; sampling techniques. Structure elucidation through interpretation of data. Effect and importance of isotope substitution.

Flame Atomic Absorption and Emission Spectrometry: Basic principles of instrumentation (choice of source, monochromator, and detector, choice of flame and Burner designs. Techniques of atomization and sample introduction. Method of background correction, sources of chemical interferences and their method of removal. Techniques for the quantitative estimation of trace level of metal ions from water samples.

Thermal methods of analysis:

Theory of thermogravimetry (TG), basic principle of instrumentation.

Techniques for quantitative estimation of Ca and Mg from their mixture.

Electroanalytical methods:

Classification of electroanalytical methods, basic principle of pH metric, potentiometric and conductometric titrations. Techniques used for the determination of equivalence points.

Techniques used for the determination of pKa values.

Separation techniques:

Solvent extraction: Classification, principle and efficiency of the technique.

Mechanism of extraction: extraction by solvation and chelation.

Technique of extraction: batch, continuous and counter current extractions.

Qualitative and quantitative aspects of solvent extraction: extraction of metal ions from aqueous solution, extraction of organic species from the aqueous and nonaqueous media.

Chromatography: Classification, principle and efficiency of the technique.

Mechanism of separation: adsorption, partition & ion exchange.

Development of chromatograms: frontal, elution and displacement methods.

Qualitative and quantitative aspects of chromatographic methods of analysis: IC, GLC, GPC, TLC and HPLC.

Stereoisomeric separation and analysis: Measurement of optical rotation, calculation of Enantiomeric excess (ee)/ diastereomeric excess (de) ratios and determination of enantiomeric composition using NMR, Chiral solvents and chiral shift reagents. Chiral chromatographic techniques using chiral columns (GC and HPLC).

Role of computers in instrumental methods of analysis.

Recommended Books:

1. Mendham, J. et al.: Vogel's Text Book of Quantitative Chemical Analysis ; 6th Ed. Pearson Education, 2009.
2. Willard, Hobert H. et al.: Instrumental Methods of Analysis, 7th Ed. CBS Publishers & Distributors, 2004.
3. Christian, Gary D: Analytical Chemistry, 6th Ed. Wiley India (P) Ltd., 2004.
4. Harris, Daniel C: Exploring Chemical Analysis, 4th Ed. W. H. Freeman, 2008.
5. Khopkar, S.M.: Basic Concepts of Analytical Chemistry, 3rd Ed. New Age, International Publisher, 2009.
6. Skoog, D.A. Holler F.J. and Nieman, T.A. Principles of Instrumental Analysis, 6th Ed. Thomson Asia Pvt. Ltd. Singapore.
7. Mikes, O. and Chalmes, R.A. Laboratory Hand Book of Chromatographic & Allied

Methods, Elles Harwood Ltd. London.1979

8. Ditts, R.V. *Analytical Chemistry: Methods of separation*. Van Nostrand, New York, 1974.

CHE-HE-5024: Lab

60 Lectures

1. Separation Techniques

I. Chromatography:

(a) Separation of mixtures

(i) Paper chromatographic separation of Fe^{3+} , Al^{3+} , and Cr^{3+} .

(ii) Separation and identification of the monosaccharides present in the given mixture (glucose & fructose) by paper chromatography. Reporting the R_f values.

(b) Separate a mixture of Sudan yellow and Sudan Red by TLC technique and identify them on the basis of their R_f values.

(c) Chromatographic separation of the active ingredients of plants, flowers and juices by TLC

II. Solvent Extractions:

(i) To separate a mixture of Ni^{2+} & Fe^{2+} by complexation with DMG and extracting the Ni^{2+} - DMG complex in chloroform, and determine its concentration by spectrophotometry.

(ii) Solvent extraction of zirconium with amberliti LA-1, separation from a mixture of irons and gallium.

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3. Determine the pH of the given aerated drinks fruit juices, shampoos and soaps.

4. Determination of Na, Ca, Li in cola drinks and fruit juices using flame photometric techniques.

5. Analysis of soil:

(i) Determination of pH of soil.

(ii) Total soluble salt

(iii) Estimation of calcium, magnesium, phosphate, nitrate

6. Ion exchange:

(i) Determination of exchange capacity of cation exchange resins and anion exchange resins.

(ii) Separation of metal ions from their binary mixture.

(iii) Separation of amino acids from organic acids by ion exchange chromatography.

7. Spectrophotometry

(i) Determination of pK_a values of indicator using spectrophotometry.

(ii) Structural characterization of compounds by infrared spectroscopy.

(iii) Determination of dissolved oxygen in water.

(iv) Determination of chemical oxygen demand (COD).

(v) Determination of Biological oxygen demand (BOD).

(vi) Determine the composition of the Ferric-salicylate/ ferric-thiocyanate complex by Job's method.

Recommended Books:

1. Vogel, Arthur I: A Test book of Quantitative Inorganic Analysis (Rev. by G.H. Jeffery and others) 5th Ed. The English Language Book Society of Longman .

2. Willard, Hobert H. et al.: Instrumental Methods of Analysis, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.

3. Christian, Gary D; Analytical Chemistry, 6th Ed. John Wiley & Sons, New York, 2004.

4. Harris, Daniel C: Exploring Chemical Analysis, Ed. New York, W.H. Freeman, 2001.

5. Khopkar, S.M. Basic Concepts of Analytical Chemistry. New Age, International Publisher, 2009.

6. Skoog, D.A. Holler F.J. and Nieman, T.A. Principles of Instrumental Analysis,

Thomson Asia Pvt. Ltd. Singapore.

7. Mikes, O. & Chalmes, R.A. Laboratory Hand Book of Chromatographic & Allied Methods, Elles Harwood Ltd. London.

9. Ditts, R.V. *Analytical Chemistry: Methods of separation*. Van Nostrand, New York, 1974.

CHE-HE-5034: MOLECULAR MODELLING & DRUG DESIGN

(Credits: Theory-04, Practicals-02)

Course Objective: *The course introduces students to the basic principles of computer assisted drug design, modelling and the important theoretical concepts and programming.*

Learning Outcome: *Students will be able to identify basic components of computer and programming as applied to computer assisted design and modelling of molecules.*

Introduction to Molecular Modelling:

Introduction. Useful Concepts in Molecular Modelling: Coordinate Systems. Potential Energy Surfaces. Molecular Graphics. Surfaces. Computer Hardware and Software. The Molecular Modelling Literature.

Force Fields:

Fields. Bond Stretching. Angle Bending. Introduction to nonbonded interactions. Electrostatic interactions. van der Waals Interactions. Hydrogen bonding in Molecular Mechanics. Force Field Models for the Simulation of Liquid Water.

Energy Minimization and Computer Simulation:

Minimization and related methods for exploring the energy surface. Non-derivative method, First and second order minimization methods. Computer simulation methods. Simple thermodynamic properties and Phase Space. Boundaries. Analyzing the results of a simulation and estimating Errors.

Molecular Dynamics & Monte Carlo Simulation:

Molecular Dynamics Simulation Methods. Molecular Dynamics using simple models. Molecular Dynamics with continuous potentials. Molecular Dynamics at constant temperature and pressure. Metropolis method. Monte Carlo simulation of molecules. Models used in Monte Carlo simulations of polymers.

Structure Prediction and Drug Design:

Structure prediction - Introduction to comparative Modeling. Sequence alignment. Constructing and evaluating a comparative model. Predicting protein structures by 'Threading', Molecular docking. Structure based de novo ligand design, Drug Discovery – Chemoinformatics – QSAR.

Recommended Books:

1. A.R. Leach, *Molecular Modelling Principles and Application*, Longman, 2001.
 2. J.M. Haile, *Molecular Dynamics Simulation Elementary Methods*, John Wiley and Sons, 1997.
 3. Satya Prakash Gupta, *QSAR and Molecular Modeling*, Springer - Anamaya Publishers, 2008.
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CHE-HE-5034: Lab

- i. Compare the optimized C-C bond lengths in ethane, ethene, ethyne and benzene. Visualize the molecular orbitals of the ethane σ bonds and ethene, ethyne, benzene and pyridine π bonds.

- ii. (a) Perform a conformational analysis of butane. (b) Determine the enthalpy of isomerization of *cis* and *trans* 2-butene.
- iii. Visualize the electron density and electrostatic potential maps for LiH, HF, N₂, NO and CO and comment. Relate to the dipole moments. Animate the vibrations of these molecules.
- iv. (a) Relate the charge on the hydrogen atom in hydrogen halides with their acid character. (b) Compare the basicities of the nitrogen atoms in ammonia, methylamine, dimethylamine and trimethylamine.
- v. (a) Compare the shapes of the molecules: 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol. Note the dipole moment of each molecule. (b) Show how the shapes affect the trend in boiling points: (118 °C, 100 °C, 108 °C, 82 °C, respectively).
- vi. Build and minimize organic compounds of your choice containing the following functional groups. Note the dipole moment of each compound: (a) alkyl halide (b) aldehyde (c) ketone (d) amine (e) ether (f) nitrile (g) thiol (h) carboxylic acid (i) ester (j) amide.
- vii. (a) Determine the heat of hydration of ethylene. (b) Compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.
- viii. Arrange 1-hexene, 2-methyl-2-pentene, (*E*)-3-methyl-2-pentene, (*Z*)-3-methyl-2-pentene, and 2,3-dimethyl-2-butene in order of increasing stability.
- ix. (a) Compare the optimized bond angles H₂O, H₂S, H₂Se. (b) Compare the HAH bond angles for the second row dihydrides and compare with the results from qualitative MO theory.

Note: Software: ChemSketch, ArgusLab (www.planaria-software.com), TINKER 6.2 (dasher.wustl.edu/ffe), WebLab Viewer, Hyperchem, or any similar software.

Recommended Books:

1. A.R. Leach, Molecular Modelling Principles and Application, Longman, 2001.
2. J.M. Haile, Molecular Dynamics Simulation Elementary Methods, John Wiley and Sons, 1997.
3. Satya Prakash Gupta, QSAR and Molecular Modeling, Springer - Anamaya Publishers, 2008.

CHE-HE-5044: NOVEL INORGANIC SOLIDS

(Credits: Theory-04, Practicals-02)

Course Objective: *This introductory course intends to make learners familiar with a wide variety of technologically important and emerging materials. It will prepare the learners for studying materials further at the master's level. Prior completion of one introductory UG level course on inorganic and physical chemistry will be essential.*

Learning outcome: *After the completion of this course it will also be possible for the students to opt for studying an interdisciplinary master's programme with an emphasis on the synthesis and applications of various materials or take up a job in the materials production and/or processing industry.*

Synthesis and modification of inorganic solids:

Conventional heat and beat methods, Co-precipitation method, Sol-gel methods, Hydrothermal method, Ion-exchange and Intercalation methods.

Inorganic solids of technological importance:

Solid electrolytes – Cationic, anionic, mixed Inorganic pigments – coloured solids, white and black pigments.

Molecular material and fullerenes, molecular materials & chemistry – one-dimensional metals, molecular magnets, metal containing liquid crystals.

Nanomaterials:

Overview of nanostructures and nanomaterials: classification.

Preparation of gold and silver metallic nanoparticles, self-assembled nanostructures-control of nanoarchitecture-one dimensional control. Carbon nanotubes and inorganic nanowires.

Bio-inorganic nanomaterials, DNA and nanomaterials, natural and artificial nanomaterials, bionano composites.

Introduction to engineering materials for mechanical construction:

Composition, mechanical and fabricating characteristics and applications of various types of cast irons, plain carbon and alloy steels, copper, aluminium and their alloys like duralumin, brasses and bronzes cutting tool materials, super alloys thermoplastics, thermosets and composite materials.

Composite materials:

Introduction, limitations of conventional engineering materials, role of matrix in composites, classification, matrix materials, reinforcements, metal-matrix composites, polymer-matrix composites, fibre-reinforced composites, environmental effects on composites, applications of composites.

Speciality polymers:

Ceramics & Refractory: Introduction, classification, properties, raw materials, manufacturing and applications.

Recommended Books:

1. Shriver & Atkins. Inorganic Chemistry, Peter Atkins, Tina Overton, Jonathan Rourke, Mark Weller and Fraser Armstrong, 5th Edition, Oxford University Press (2011-2012)
2. Smart, L. E., Moore, E. A., Solid State Chemistry: An Introduction, 4th Ed., CRC Press, 2012.
3. Poole, C. P., Owens, F. J., Introduction to Nanotechnology, Wiley India, 2009.
4. Murty, B. S., Shankar, P., Raj, B., Rath, B. B., Murday, J. Textbook of Nanoscience and Nanotechnology, Springer, 2013.

CHE-HE-5044: Lab

1. Determination of cation exchange capacity.
2. Synthesis of oxides by ceramic method.
3. Synthesis of hydrogel by co-precipitation method.
4. Synthesis of silver and gold metal nanoparticles.

Recommended Book:

1. Fahlman, B. D., Materials *Chemistry*, Springer (2011).
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CHE-HE-5054: POLYMER CHEMISTRY

(Credits: Theory-06, Practicals-02)

Course objective: This is an introductory level course in polymer chemistry. The aim of the course is to introduce the theory and applications of polymer chemistry to the students.

Some industrially important polymers and conducting polymers, a promising class of polymeric materials for next generation devices will also be introduced in this course.

Learning outcome: After completion of this course the students will learn the definition and classifications of polymers, kinetics of polymerization, molecular weight of polymers, glass

transition temperature, and polymer solutions etc. They also learn the brief introduction of preparation, structure and properties of some industrially important and technologically promising polymers.

Introduction and history of polymeric materials:

Different schemes of classification of polymers, Polymer nomenclature, Molecular forces and chemical bonding in polymers, Texture of Polymers.

Functionality and its importance:

Criteria for synthetic polymer formation, classification of polymerization processes, Relationships between functionality, extent of reaction and degree of polymerization. Bifunctional systems, Poly-functional systems.

Kinetics of Polymerization:

Mechanism and kinetics of step growth, radical chain growth, ionic chain (both cationic and anionic) and coordination polymerizations, Mechanism and kinetics of copolymerization, polymerization techniques.

Crystallization and crystallinity:

Determination of crystalline melting point and degree of crystallinity, Morphology of crystalline polymers, Factors affecting crystalline melting point.

Nature and structure of polymers-Structure Property relationships.

Determination of molecular weight of polymers (M_n , M_w , etc) by end group analysis, viscometry, light scattering and osmotic pressure methods. Molecular weight distribution and its significance. Polydispersity index.

Glass transition temperature (T_g) and determination of T_g, Free volume theory, WLF equation, Factors affecting glass transition temperature (T_g).

Polymer Solution – Criteria for polymer solubility, Solubility parameter, Thermodynamics of polymer solutions, entropy, enthalpy, and free energy change of mixing of polymers solutions, Flory- Huggins theory, Lower and Upper critical solution temperatures.

Properties of Polymers (Physical, thermal, Flow & Mechanical Properties).

Brief introduction to preparation, structure, properties and application of the following polymers: polyolefins, polystyrene and styrene copolymers, poly(vinyl chloride) and related polymers, poly(vinyl acetate) and related polymers, acrylic polymers, fluoro polymers, polyamides and related polymers. Phenol formaldehyde resins (Bakelite, Novalac), polyurethanes, silicone polymers, polydienes, Polycarbonates, Conducting Polymers, [polyacetylene, polyaniline, poly(p-phenylene sulphide polypyrrole, polythiophene)].

Recommended Books:

1. Seymour's *Polymer Chemistry*, Marcel Dekker, Inc.
2. G. Odian: *Principles of Polymerization*, John Wiley.
3. F.W. Billmeyer: *Text Book of Polymer Science*, John Wiley.
4. P. Ghosh: *Polymer Science & Technology*, Tata McGraw-Hill.
5. R.W. Lenz: *Organic Chemistry of Synthetic High Polymers*.

1. Polymer synthesis

1. Free radical solution polymerization of styrene (St) / Methyl Methacrylate (MMA) / Methyl Acrylate (MA) / Acrylic acid (AA).

a. Purification of monomer

b. Polymerization using benzoyl peroxide (BPO) / 2,2'-azo-bis-isobutyronitrile (AIBN)

2. Preparation of nylon 66/6

1. Interfacial polymerization, preparation of polyester from isophthaloyl chloride (IPC) and phenolphthalein

a. Preparation of IPC

b. Purification of IPC

c. Interfacial polymerization

3. Redox polymerization of acrylamide

4. Precipitation polymerization of acrylonitrile

5. Preparation of urea-formaldehyde resin

6. Preparations of novalac resin/resold resin.

7. Microscale Emulsion Polymerization of Poly(methylacrylate).

Polymer characterization

1. Determination of molecular weight by viscometry:

(a) Polyacrylamide-aq. NaNO₂ solution

(b) (Poly vinyl propylidene (PVP) in water

2. Determination of the viscosity-average molecular weight of poly(vinyl alcohol) (PVOH) and the fraction of "head-to-head" monomer linkages in the polymer.

3. Determination of molecular weight by end group analysis: Polyethylene glycol (PEG) (OH group).

4. Testing of mechanical properties of polymers.

5. Determination of hydroxyl number of a polymer using colorimetric method.

Polymer analysis

1. Estimation of the amount of HCHO in the given solution by sodium sulphite method

2. Instrumental Techniques

3. IR studies of polymers

4. DSC analysis of polymers

5. Preparation of polyacrylamide and its electrophoresis

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*at least 7 experiments to be carried out.

Recommended Books:

1. Malcolm P. Stevens, Polymer Chemistry: An Introduction, 3rd Ed.

2. Harry R. Allcock, Frederick W. Lampe and James E. Mark, Contemporary Polymer Chemistry, 3rd ed. Prentice-Hall (2003)

3. Fred W. Billmeyer, Textbook of Polymer Science, 3rd ed. Wiley-Interscience (1984)

4. Joel R. Fried, Polymer Science and Technology, 2nd ed. Prentice-Hall (2003)

5. Petr Munk and Tejraj M. Aminabhavi, Introduction to Macromolecular Science, 2nd ed. John Wiley & Sons (2002)

6. L. H. Sperling, Introduction to Physical Polymer Science, 4th ed. John Wiley & Sons (2005)

7. Malcolm P. Stevens, Polymer Chemistry: An Introduction, 3rd ed. Oxford University Press (2005)

8. Seymour/ Carraher's Polymer Chemistry, 9th ed. by Charles E. Carraher, Jr. (2013).

. CHE-HE-6046: RESEARCH METHODOLOGY FOR CHEMISTRY

(Credits: Theory-05, Tutorials-01)

Course Objectives:

This course is introduced to impart knowledge about the basic concepts of research and to provide a road map for conducting research

Students are expected to identify, explain and apply basic concepts of research; acquire information, recognize various issues related to research and to learn instrumental methods required for research in chemistry.

Learning Outcome:

After completing this course, students should be able to construct a rational research proposal to generate fruitful output in terms of publications and patents in the field of chemical sciences.

Literature Survey:

Print: Sources of information: Primary, secondary, tertiary sources; Journals: Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text-books, current contents, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples.

Digital: Web resources, E-journals, Journal access, TOC alerts, Hot articles, Citation index, Impact factor, H-index, E-consortium, UGC infonet, E-books, Internet discussion groups and communities, Blogs, Preprint servers, Search engines, Scirus, Google Scholar, ChemIndustry, Wiki- Databases, ChemSpider, Science Direct, SciFinder, Scopus.

Information Technology and Library Resources: The Internet and World Wide Web. Internet resources for chemistry. Finding and citing published information.

Methods of Scientific Research and Writing Scientific Papers:

Reporting practical and project work. Writing literature surveys and reviews. Organizing a poster display. Giving an oral presentation.

Writing scientific papers – justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work.

Writing ethics. Avoiding plagiarism.

Chemical Safety and Ethical Handling of Chemicals:

Safe working procedure and protective environment, protective apparel, emergency procedure and first aid, laboratory ventilation. Safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmospheric – safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives, identification, verification and segregation of laboratory waste, disposal of chemicals in the sanitary sewer system, incineration and transportation of hazardous chemicals.

Data Analysis

The Investigative Approach: Making and Recording Measurements. SI Units and their use. Scientific method and design of experiments.

Analysis and Presentation of Data: Descriptive statistics. Choosing and using statistical tests. Chemometrics. Analysis of variance (ANOVA), Correlation and regression, Curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, General polynomial fitting, linearizing transformations, exponential function fit, r and its abuse. Basic aspects of multiple linear regression analysis.

Electronics

Basic fundamentals of electronic circuits and their components used in circuits of common

instruments like spectrophotometers, typical circuits involving operational amplifiers for electrochemical instruments. Elementary aspects of digital electronics.

Recommended Books

1. Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J. & Jones, A. (2011) *Practical skills in chemistry*. 2nd Ed. Prentice-Hall, Harlow.
2. Hibbert, D. B. & Gooding, J. J. (2006) *Data analysis for chemistry*. Oxford University Press.
3. Topping, J. (1984) *Errors of observation and their treatment*. Fourth Ed., Chapman Hall, London.
4. Harris, D. C. *Quantitative chemical analysis*. 6th Ed., Freeman (2007) Chapters 3-5.
5. Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis*. Cambridge Univ. Press (2001) 487 pages.
6. Chemical safety matters – IUPAC – IPCS, Cambridge University Press, 1992.
7. OSU safety manual 1.01.

CHE-HE-6014 : GREEN CHEMISTRY

(Credits: Theory-04, Practicals-02)

Course Objective: *The learners will be taught about the emerging discipline of green chemistry particularly to differentiate as to how the principles of green chemistry may be applied to organic synthesis.*

Learning Outcome: *Apart from introducing learners to the principles of green chemistry, this course will make them conversant with applications of green chemistry to organic synthesis. Students will be prepared for taking up entry level jobs in the chemical industry. They also will have the option of studying further in the area.*

Introduction to Green Chemistry

What is Green Chemistry? Need for Green Chemistry. Goals of Green Chemistry. Limitations/ Obstacles in the pursuit of the goals of Green Chemistry.

Principles of Green Chemistry and Designing a Chemical synthesis

Twelve principles of Green Chemistry with their explanations and examples; Designing a Green Synthesis using these principles; Prevention of Waste/ byproducts; maximum incorporation of the materials used in the process into the final products (Atom Economy); prevention/ minimization of hazardous/ toxic products; designing safer chemicals – different basic approaches to do so; selection of appropriate auxiliary substances (solvents, separation agents), green solvents, solventless processes, immobilized solvents and ionic liquids; energy requirements for reactions - use of microwaves, ultrasonic energy; selection of starting materials; avoidance of unnecessary derivatization – careful use of blocking/protecting groups; use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; designing of biodegradable products; prevention of chemical accidents; strengthening/ development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

Examples of Green Synthesis/ Reactions

1. Green Synthesis of the following compounds: adipic acid, catechol, BHT, methyl methacrylate, urethane, citral, ibuprofen, paracetamol, furfural.
2. Microwave assisted reactions in water: Oxidation of toluene, alcohols. Microwave assisted

reactions in organic solvents: Esterification, Fries rearrangement, Diels-Alder Reaction. Microwave assisted solid state reactions: Deacetylation, Deprotection. Saponification of esters, Alkylation of reactive methylene compounds, reductions, benzimidazoles.
3. Selective methylation of active methylene group using dimethylcarbonate: Solid-state polymerization of amorphous polymers using diphenylcarbonate; Use of "Clayan", a nonmetallic oxidative reagent for various reactions; Free Radical Bromination; Role of Tellurium in organic syntheses; Biocatalysis in organic syntheses.

Future Trends in Green Chemistry

Oxidation reagents and catalysts; Biomimetic, multifunctional reagents; Solventless reactions; Green chemistry in sustainable development.

Recommended Books:

1. V.K. Ahluwalia & M.R. Kidwai: New Trends in Green Chemistry, Anamalaya Publishers (2005).
2. P.T. Anastas & J.K. Warner: Oxford Green Chemistry- Theory and Practical, University Press (1998).
3. A.S. Matlack: Introduction to Green Chemistry, Marcel Dekker (2001).
4. M.C. Cann & M.E. Connelly: Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).
5. M.A. Ryan & M. Tinnesand, Introduction to Green Chemistry, American Chemical Society, Washington (2002).

CHE-HE-6014: Lab

1. Safer starting materials

The Vitamin C clock reaction using Vitamin C tablets, tincture of iodine, hydrogen peroxide and liquid laundry starch.

- (i) Effect of concentration on clock reaction
- (ii) Effect of temperature on clock reaction.

2. Using renewable resources

Preparation of biodiesel from vegetable oil.

3. Avoiding waste

Principle of atom economy.

Use of molecular model kit to stimulate the reaction to investigate how the atom economy can illustrate Green Chemistry.

Preparation of propene by two methods can be studied

(I) Triethylamine ion + OH⁻

→ propene + trimethylpropene + water

(II) 1-propanol propene + water

The other types of reactions, like addition, elimination, substitution and rearrangement should also be studied for the calculation of atom economy.

4. Use of enzymes as catalysts

Benzoin condensation using Thiamine Hydrochloride as a catalyst instead of cyanide

Alternative Green solvents

5. Diels Alder reaction in water

Reaction between furan and maleic acid in water and at room temperature rather than in benzene and reflux.

6. Extraction of D-limonene from orange peel using liquid CO₂ prepared from dry ice.

7. Mechanochemical solvent free synthesis of azomethines

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8. Co-crystal controlled solid state synthesis (C₂S₃) of N-organophthalimide using phthalic anhydride and 3-aminobenzoic acid.

Alternative sources of energy

9. Solvent free, microwave assisted one pot synthesis of phthalocyanine complex of copper (II).

10. Photoreduction of benzophenone to benzopinacol in the presence of sunlight.

Recommended Books:

1. Anastas, P.T & Warner, J.C. *Green Chemistry: Theory and Practice*, Oxford University Press (1998).
2. Kirchoff, M. & Ryan, M.A. *Greener approaches to undergraduate chemistry experiment*. American Chemical Society, Washington DC (2002).
3. Ryan, M.A. *Introduction to Green Chemistry*, Tinnensand; (Ed), American Chemical Society, Washington DC (2002).
4. Sharma, R.K.; Sidhwani, I.T. & Chaudhari, M.K. *Green Chemistry Experiment: A monograph*, I.K International Publishing House Pvt Ltd. New Delhi. Bangalore CISBN 978-93-81141-55-7 (2013).
5. Cann, M.C. & Connelly, M. E. *Real world cases in Green Chemistry*, American Chemical Society (2008).
6. Cann, M. C. & Thomas, P. *Real world cases in Green Chemistry*, American Chemical Society (2008).
7. Pavia, D. L. Lampman, G. H. & Kriz, G.S. *W B Introduction to Organic Laboratory Techniques: A Microscale Approach*, 4th Ed., Brooks/Cole; 2007.

CHE-HE-6024: INDUSTRIAL CHEMICALS AND ENVIRONMENT

(Credits: Theory-04, Practicals-02)

Course Objectives: *This course provides an introduction to the various industrial gases and inorganic chemicals, their manufacturing processes, applications, storage and the hazards of handling them. Contribution of these industrial chemicals towards air and water pollution and their effects on living organisms and the environment has also been covered. Students are also expected to learn about metallurgy, energy generation industry and the pollution threat they pose. This course also discusses about management of the different kinds of wastes, their safe disposal and the importance of practicing green chemistry in chemical industry.*

Learning Outcomes: *After successful completion of the course, students would have learnt about the manufacture, applications and safe ways of storage and handling gaseous and inorganic industrial chemicals. Students will get to know about industrial metallurgy and the energy generation industry. Students will also learn about environmental pollution by various gaseous, liquid wastes and nuclear wastes and their effects on living beings. Finally, the students will learn about industrial waste management, their safe disposal and the importance of environment friendly “green chemistry” in chemical industry.*

Industrial Gases and Inorganic Chemicals

Industrial Gases: Large scale production, uses, storage and hazards in handling of the following gases: oxygen, nitrogen, argon, neon, helium, hydrogen, acetylene, carbon monoxide, chlorine, fluorine, sulphur dioxide and phosgene.

Inorganic Chemicals: Manufacture, application, analysis and hazards in handling the following chemicals: hydrochloric acid, nitric acid, sulphuric acid, caustic soda, common salt, borax, bleaching powder, sodium thiosulphate, hydrogen peroxide, potash alum, chrome alum, potassium dichromate and potassium permanganate.

Industrial Metallurgy

Preparation of metals (ferrous and nonferrous) and ultrapure metals for semiconductor

technology.

Environment and its segments

Ecosystems. Biogeochemical cycles of carbon, nitrogen and sulphur.

Air Pollution: Major regions of atmosphere. Chemical and photochemical reactions in atmosphere. Air pollutants: types, sources, particle size and chemical nature; Photochemical smog: its constituents and photochemistry. Environmental effects of ozone, Major sources of air pollution.

Pollution by SO₂, CO₂, CO, NO_x, H₂S and other foul smelling gases. Methods of estimation of CO, NO_x, SO_x and control procedures.

Effects of air pollution on living organisms and vegetation. Greenhouse effect and Global warming, Ozone depletion by oxides of nitrogen, chlorofluorocarbons and Halogens, removal of sulphur from coal. Control of particulates.

Water Pollution: Hydrological cycle, water resources, aquatic ecosystems, Sources and nature of water pollutants, Techniques for measuring water pollution, Impacts of water pollution on hydrological and ecosystems.

Water purification methods. Effluent treatment plants (primary, secondary and tertiary treatment). Industrial effluents from the following industries and their treatment: electroplating, textile, tannery, dairy, petroleum and petrochemicals, agro, fertilizer, etc. Sludge disposal.

Industrial waste management, incineration of waste. Water treatment and purification (reverse osmosis, electro dialysis, ion exchange). Water quality parameters for waste water, industrial water and domestic water.

Energy & Environment

Sources of energy: Coal, petrol and natural gas. Nuclear Fusion / Fission, Solar energy, Hydrogen, geothermal, Tidal and Hydel, etc.

Nuclear Pollution: Disposal of nuclear waste, nuclear disaster and its management.

(10 Lectures)

Biocatalysis

Introduction to biocatalysis: Importance in “Green Chemistry” and Chemical Industry.

(6 Lectures)

Recommended Books:

1. E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK.
2. R.M. Felder, R.W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi.
3. J. A. Kent: *Riegel's Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.
4. S. S. Dara: *A Textbook of Engineering Chemistry*, S. Chand & Company Ltd. New Delhi.
5. K. De, *Environmental Chemistry*: New Age International Pvt., Ltd, New Delhi.
6. S. M. Khopkar, *Environmental Pollution Analysis*: Wiley Eastern Ltd, New Delhi.
7. S.E. Manahan, *Environmental Chemistry*, CRC Press (2005).
8. G.T. Miller, *Environmental Science* 11th edition. Brooks/ Cole (2006).
9. A. Mishra, *Environmental Studies*. Selective and Scientific Books, New Delhi (2005).

CHE-HE-6024: Lab

1. Determination of dissolved oxygen in water.
2. Determination of Chemical Oxygen Demand (COD)
3. Determination of Biological Oxygen Demand (BOD)
4. Percentage of available chlorine in bleaching powder.

5. Measurement of chloride, sulphate and salinity of water samples by simple titration method (AgNO_3 and potassium chromate).
6. Estimation of total alkalinity of water samples (CO_3^{2-} , HCO_3^-) using double titration method.
7. Measurement of dissolved CO_2 .
8. Study of some of the common bio-indicators of pollution.
9. Estimation of SPM in air samples.
10. Preparation of borax/ boric acid.

Recommended Books:

1. E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK.
2. R.M. Felder, R.W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi.
3. J. A. Kent: Riegel's *Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.
4. S. S. Dara: *A Textbook of Engineering Chemistry*, S. Chand & Company Ltd. New Delhi.
5. K. De, *Environmental Chemistry*: New Age International Pvt., Ltd, New Delhi.
6. S. M. Khopkar, *Environmental Pollution Analysis*: Wiley Eastern Ltd, New Delhi.

CHE-HE-6034: INORGANIC MATERIALS OF INDUSTRIAL IMPORTANCE

(Credits: Theory-04, Practicals-02)

Course Objectives: To learn the synthetic process, properties and the utility of the industrially important inorganic materials (such as silicates, ceramics, cements, fertilizers, paints, batteries, alloys and explosives).

To provide opportunity to learn some of the industrial process such as surface coating and catalysis in relevant to industry where heterogeneous catalysis dominates.

Experiments are aimed at helping learners acquire hands on experience in qualitative and quantitative analysis of the inorganic materials which are basically manufactured in chemical industries.

To learn some industrial techniques such as surface coating etc..

Learning Outcome: This course will establish the basic foundation of industrial inorganic chemistry among the students. This will be helpful for pursuing further studies of industrial chemistry in future. Experiments will help the Students to gather the experience of qualitative and quantitative chemical analysis. Students will be capable of doing analysis of the inorganic materials which are used in our daily life. They will have insight of the industrial processes.

Silicate Industries

Glass: Glassy state and its properties, classification (silicate and non-silicate glasses).

Manufacture and processing of glass. Composition and properties of the following types of glasses: Soda lime glass, lead glass, armoured glass, safety glass, borosilicate glass, fluorosilicate, coloured glass, photosensitive glass.

Ceramics: Important clays and feldspar, ceramic, their types and manufacture. High technology ceramics and their applications, superconducting and semiconducting oxides, fullerenes carbon nanotubes and carbon fibre.

Cements: Classification of cement, ingredients and their role, Manufacture of cement and the setting process, quick setting cements.

Fertilizers:

Different types of fertilizers. Manufacture of the following fertilizers: Urea, ammonium

nitrate, calcium ammonium nitrate, ammonium phosphates; polyphosphate, superphosphate, compound and mixed fertilizers, potassium chloride, potassium sulphate.

Surface Coatings:

Objectives of coatings surfaces, preliminary treatment of surface, classification of surface coatings. Paints and pigments-formulation, composition and related properties. Oil paint, Vehicle, modified oils, Pigments, toners and lakes pigments, Fillers, Thinners, Enamels, emulsifying agents. Special paints (Heat retardant, Fire retardant, Eco-friendly paint, Plastic paint), Dyes, Wax polishing, Water and Oil paints, additives, Metallic coatings (electrolytic and electroless), metal spraying and anodizing.

Batteries:

Primary and secondary batteries, battery components and their role, Characteristics of battery. Working of following batteries: Pb acid, Li-Battery, Solid state electrolyte battery. Fuel cells, Solar cell and polymer cell.

Alloys:

Classification of alloys, ferrous and non-ferrous alloys, Specific properties of elements in alloys. Manufacture of Steel (removal of silicon decarbonization, demanganization, desulphurization dephosphorisation) and surface treatment (argon treatment, heat treatment, nitriding, carburizing). Composition and properties of different types of steels.

Catalysis:

General principles and properties of catalysts, homogenous catalysis (catalytic steps and examples) and heterogenous catalysis (catalytic steps and examples) and their industrial applications, Deactivation or regeneration of catalysts. Phase transfer catalysts, application of zeolites as catalysts.

Chemical explosives:

Origin of explosive properties in organic compounds, preparation and explosive properties of lead azide, PETN, cyclonite (RDX). Introduction to rocket propellants.

Recommended Books:

1. E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK.
2. R. M. Felder, R. W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi.
3. W. D. Kingery, H. K. Bowen, D. R. Uhlmann: *Introduction to Ceramics*, Wiley Publishers, New Delhi.
4. Karl Heinz Büchel, Hans-Heinrich Moretto Peter, Woditsch; *Industrial Inorganic Chemistry*, Wiley-VCH.
5. J. A. Kent: Riegel's *Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.
6. P. C. Jain, M. Jain: *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.
7. R. Gopalan, D. Venkappayya, S. Nagarajan: *Engineering Chemistry*, Vikas Publications, New Delhi.
8. B. K. Sharma: *Engineering Chemistry*, Goel Publishing House, Meerut

CHE-HE-6034: Lab

1. Determination of free acidity in ammonium sulphate fertilizer.
2. Estimation of Calcium in Calcium ammonium nitrate fertilizer.
3. Estimation of phosphoric acid in superphosphate fertilizer.
4. Electroless metallic coatings on ceramic and plastic material.
5. Determination of composition of dolomite (by complexometric titration).

6. Analysis of (Cu, Ni); (Cu, Zn) in alloy or synthetic samples.
7. Analysis of Cement.
8. Preparation of pigment (zinc oxide).

Recommended Books:

1. E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK.
 2. R. M. Felder, R. W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi.
 3. W. D. Kingery, H. K. Bowen, D. R. Uhlmann: *Introduction to Ceramics*, Wiley Publishers, New Delhi.
 4. J. A. Kent: Riegel's *Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.
 5. P. C. Jain, M. Jain: *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.
 6. R. Gopalan, D. Venkappayya, S. Nagarajan: *Engineering Chemistry*, Vikas Publications, New Delhi.
 7. B. K. Sharma: *Engineering Chemistry*, Goel Publishing House, Meerut
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CHE-HE-5064: INSTRUMENTAL METHODS OF CHEMICAL ANALYSIS**(Credits: Theory-04, Practicals-02)**

Course Objective: Students shall be introduced to the fundamental concepts/theory and application of different analytical techniques, as applied to chemistry.

Learning Outcome: Students shall be able to explain the theoretical basis of different analytical techniques, identify the experimental requirements and compare/analyze the data/results thereof.

Introduction to spectroscopic methods of analysis:

Recap of the spectroscopic methods covered in detail in the core chemistry syllabus: Treatment of analytical data, including error analysis. Classification of analytical methods and the types of instrumental methods. Consideration of electromagnetic radiation.

Molecular spectroscopy:

Infrared spectroscopy:

Interactions with molecules: absorption and scattering. Means of excitation (light sources), separation of spectrum (wavelength dispersion, time resolution), detection of the signal (heat, differential detection), interpretation of spectrum (qualitative, mixtures, resolution), advantages of Fourier Transform (FTIR). Samples and results expected. Applications: Issues of quality assurance and quality control, Special problems for portable instrumentation and rapid detection.

UV-Visible/ Near IR – emission, absorption, fluorescence and photoacoustic. Excitation sources (lasers, time resolution), wavelength dispersion (gratings, prisms, interference filters, laser, placement of sample relative to dispersion, resolution), Detection of signal (photocells, photomultipliers, diode arrays, sensitivity and S/N), Single and Double Beam instruments, Interpretation (quantification, mixtures, absorption vs. fluorescence and the use of time, photoacoustic, fluorescent tags).

Separation techniques

Chromatography: Gas chromatography, liquid chromatography, supercritical fluids, Importance of column technology (packing, capillaries), Separation based on increasing number of factors (volatility, solubility, interactions with stationary phase, size, electrical

field), Detection: simple vs. specific (gas and liquid), Detection as a means of further analysis (use of tags and coupling to IR and MS), Electrophoresis (plates and capillary) and use with DNA analysis.

Immunoassays and DNA techniques

Mass spectroscopy: Making the gaseous molecule into an ion (electron impact, chemical ionization), Making liquids and solids into ions (electrospray, electrical discharge, laser desorption, fast atom bombardment), Separation of ions on basis of mass to charge ratio, Magnetic, Time of flight, Electric quadrupole. Resolution, time and multiple separations, Detection and interpretation (how this is linked to excitation).

Elemental analysis:

Mass spectrometry (electrical discharges).

Atomic spectroscopy: Atomic absorption, Atomic emission, and Atomic fluorescence
Excitation and getting sample into gas phase (flames, electrical discharges, plasmas),
Wavelength separation and resolution (dependence on technique), Detection of radiation (simultaneous/scanning, signal noise), Interpretation (errors due to molecular and ionic species, matrix effects, other interferences).

NMR spectroscopy: Principle, Instrumentation, Factors affecting chemical shift, Spincoupling, Applications.

Electroanalytical Methods: Potentiometry & Voltammetry

Radiochemical Methods

X-ray analysis and electron spectroscopy (surface analysis)

Recommended books:

1. Principles of Instrumental Analysis - 6th Edition by Douglas A. Skoog, F. James Holler, and Stanley Crouch (ISBN 0-495-01201-7).
2. Instrumental Methods of Analysis, 7th ed, Willard, Merritt, Dean, Settle. 64
3. P.W. Atkins: Physical Chemistry.
4. G.W. Castellan: Physical Chemistry.
5. C.N. Banwell: Fundamentals of Molecular Spectroscopy.
6. Brian Smith: Infrared Spectral Interpretations: A Systematic Approach.
7. W.J. Moore: Physical Chemistry.

CHE-HE-5064: Lab

1. Safety Practices in the Chemistry Laboratory
2. Determination of the isoelectric pH of a protein.
3. Titration curve of an amino acid.
4. Determination of the void volume of a gel filtration column.
5. Determination of a Mixture of Cobalt and Nickel (UV/Vis spec.)
6. Study of Electronic Transitions in Organic Molecules (i.e., acetone in water)
7. IR Absorption Spectra (Study of Aldehydes and Ketones)
8. Determination of Calcium, Iron, and Copper in Food by Atomic Absorption
9. Quantitative Analysis of Mixtures by Gas Chromatography (i.e., chloroform and carbon tetrachloride)
10. Separation of Carbohydrates by HPLC
11. Determination of Caffeine in Beverages by HPLC
12. Potentiometric Titration of a Chloride-Iodide Mixture

13. Cyclic Voltammetry of the Ferrocyanide/Ferricyanide Couple
14. Nuclear Magnetic Resonance
15. Use of fluorescence to do “presumptive tests” to identify blood or other body fluids.
16. Use of “presumptive tests” for anthrax or cocaine
17. Collection, preservation, and control of blood evidence being used for DNA testing
18. Use of capillary electrophoresis with laser fluorescence detection for nuclear DNA (Y-chromosome only or multiple chromosome)
19. Use of sequencing for the analysis of mitochondrial DNA
20. Laboratory analysis to confirm anthrax or cocaine
21. Detection in the field and confirmation in the laboratory of flammable accelerants or explosives
22. Detection of illegal drugs or steroids in athletes
23. Detection of pollutants or illegal dumping
24. Fibre analysis

At least 10 experiments to be performed.

Recommended Books:

1. Principles of Instrumental Analysis - 6th Edition by Douglas A. Skoog, F. James Holler and Stanley Crouch (ISBN 0-495-01201-7).
2. Instrumental Methods of Analysis, 7th ed, Willard, Merritt, Dean, Settle.

Skill Enhancement Courses

CHE-SE-3024: IT SKILLS FOR CHEMISTS

(Credits: 04)

Course Objective: *The objectives of the proposed course are:*

- 1) *To provide the basic knowledge of mathematics which are needed to pursue chemistry as major subject.*
- 2) *To provide the necessary training for the basic programming knowledge.*
- 3) *The course provides information technology literacy and basic skills training for learners with limited experience.*
- 4) *To familiarize with the Introductory writing activities and Handling numeric data.*

Learning Outcome: *Course learning outcomes focus on skill development related to basic computer operations and information technology. After completing the course the incumbent is able to use the computer for basic purposes of preparing his personnel/business letters, viewing information on Internet (the web), sending mails, using internet banking services etc. After opting this course the students are expected to accumulate the skills in writing activities and Handling numeric data.*

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).

Computer programming:

Constants, variables, bits, bytes, binary and ASCII formats, arithmetic expressions, hierarchy of operations, inbuilt functions. Elements of the BASIC language. BASIC keywords and commands. Logical and relative operators. Strings and graphics. Compiled versus interpreted languages. Errors (Syntax and Logical), 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).

HANDS ON

Introductory writing activities: Introduction to word processor and structure drawing (ChemSketch) 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/Latex.

Handling numeric data: Spreadsheet software (Excel), 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, linear regression (rate constants from concentrationtime data, molar extinction coefficients from absorbance data), numerical differentiation (e.g. handling data from potentiometric and pH metric titrations, pK_a of weak acid), integration (e.g. entropy/enthalpy change from heat capacity data).

Statistical analysis: Gaussian distribution and Errors in measurements and their effect on data sets. Descriptive statistics using Excel. Statistical significance testing: The t test. The F test.

Presentation: Presentation graphics

Recommended Books:

1. McQuarrie, D. A. Mathematics for Physical Chemistry University Science Books (2008).
 2. Mortimer, R. Mathematics for Physical Chemistry. 3rd Ed. Elsevier (2005).
 3. Steiner, E. The Chemical Maths Book Oxford University Press (1996).
 4. Yates, P. Chemical calculations. 2nd Ed. CRC Press (2007).
 5. Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007) Chapters 3-5.
 6. Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis*, Cambridge Univ. Press (2001) 487 pages.
 7. Noggle, J. H. *Physical chemistry on a Microcomputer*. Little Brown & Co. (1985).
 8. Venit, S.M. *Programming in BASIC: Problem solving with structure and style*. Jaico Publishing House: Delhi (1996).
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CHE-SE-3034: BASIC ANALYTICAL CHEMISTRY

(Credits: 04)

Course Objective: To familiarize students with different micro and semimicro analytical techniques and help develop the ability to use modern instrumental methods for chemical analysis of food, soil, air and water.

Learning Outcome: Upon completion of this course, students shall be able to explain the basic principles of chemical analysis, design/implement microscale and semimicro experiments, record, interpret and analyze data following scientific methodology.

Introduction: Introduction to Analytical Chemistry and its interdisciplinary nature. Concept of sampling. Importance of accuracy, precision and sources of error in analytical measurements. Presentation of experimental data and results, from the point of view of significant figures.

Analysis of soil: Composition of soil, Concept of pH and pH measurement, Complexometric titrations, Chelation, Chelating agents, use of indicators

- Determination of pH of soil samples.
- Estimation of Calcium and Magnesium ions as Calcium carbonate by complexometric titration.

Analysis of water: Definition of pure water, sources responsible for contaminating water, water sampling methods, water purification methods.

- Determination of pH, acidity and alkalinity of a water sample.
- Determination of dissolved oxygen (DO) of a water sample.

Analysis of food products: Nutritional value of foods, idea about food processing and food preservations and adulteration.

- Identification of adulterants in some common food items like coffee powder, asafoetida, chilli powder, turmeric powder, coriander powder and pulses, etc.
- Analysis of preservatives and colouring matter.

Chromatography: Definition, general introduction on principles of chromatography, paper chromatography, TLC etc.

- Paper chromatographic separation of mixture of metal ion (Fe^{3+} and Al^{3+}).
- To compare paint samples by TLC method.

Ion-exchange: Column, ion-exchange chromatography etc.

Determination of ion exchange capacity of anion / cation exchange resin (using batch procedure if use of column is not feasible).

Analysis of cosmetics: Major and minor constituents and their function

- Analysis of deodorants and antiperspirants, Al, Zn, boric acid, chloride, sulphate.
- Determination of constituents of talcum powder: Magnesium oxide, Calcium oxide, Zinc oxide and Calcium carbonate by complexometric titration.

Suggested Applications (Any one):

- To study the use of phenolphthalein in trap cases.
- To analyze arson accelerants.
- To carry out analysis of gasoline.

Suggested Instrumental demonstrations:

- Estimation of macro nutrients: Potassium, Calcium, Magnesium in soil samples by flame photometry.
- Spectrophotometric determination of Iron in Vitamin / Dietary Tablets.
- Spectrophotometric Identification and Determination of Caffeine and Benzoic Acid in Soft Drink.

Recommended Books:

- Willard, H. H. *Instrumental Methods of Analysis*, CBS Publishers.

2. Skoog & Lerry. *Instrumental Methods of Analysis*, Saunders College Publications, New York.
 3. Skoog, D.A.; West, D.M. & Holler, F.J. *Fundamentals of Analytical Chemistry 6th Ed.*, Saunders College Publishing, Fort Worth (1992).
 4. Harris, D. C. *Quantitative Chemical Analysis*, W. H. Freeman.
 5. Dean, J. A. *Analytical Chemistry Notebook*, McGraw Hill.
 6. Day, R. A. & Underwood, A. L. *Quantitative Analysis*, Prentice Hall of India.
 7. Freifelder, D. *Physical Biochemistry 2nd Ed.*, W.H. Freeman and Co., N.Y. USA(1982).
 8. Cooper, T.G. *The Tools of Biochemistry*, John Wiley and Sons, N.Y. USA. 16(1977).
 9. Vogel, A. I. *Vogel's Qualitative Inorganic Analysis 7th Ed.*, Prentice Hall.
 10. Vogel, A. I. *Vogel's Quantitative Chemical Analysis 6th Ed.*, Prentice Hall.
 11. Robinson, J.W. *Undergraduate Instrumental Analysis 5th Ed.*, Marcel Dekker, Inc., New York (1995).
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CHE-SE-3044: CHEMICAL TECHNOLOGY & SOCIETY

(Credits: 04)

Course Objective: *The objective of the course is to enable students to have a firsthand understanding of different types of equipments needed in chemical technology and offer them concepts regarding some important parameters. The syllabus also emphasizes the dynamic nature of the relations between society on one hand and technological achievement from chemical industries on the other hand. In other words, it tries to explore societal and technological issues from a chemical perspective.*

Learning Outcome: *Students shall be familiarized with processes and terminologies in chemical industry, like mass balance, energy balance etc... Learners will be able to use chemical and scientific literacy as a means to better understand the topics related to the society.*

Chemical Technology

Different types of equipments needed in chemical technology, including reactors, distillation columns, extruders, pumps, mills, emulgators. Scaling up operations in chemical industry. Introduction to clean technology.

Concept of relative humidity, molal humidity, dew point, partial saturation.

Material Balance: Recycle, bypass in batch, stage wise and continuous operations in systems with and without chemical reactions.

Energy balance: Energy balance of systems with and without chemical reactions.

Society

Social issues related to soil, air and water pollution.

Energy crisis of modern society and search for alternatives such as energy from natural sources (i.e. solar and renewable forms), and from nuclear fission, biofuel etc.

Pros and cons of use of materials like plastics and polymers and their natural analogues,

Genetic engineering and the manufacture of drugs (proteins and nucleic acids, and molecular reactivity and interconversions)

Recommended Book:

1. John W. Hill, Terry W. McCreary & Doris K. Kolb, *Chemistry for changing times* 13th Ed.
 2. E.J. Hackett, O. Amsterdamska, M. Lynch and J. Wajcman (eds.), *The Handbook of Science and Technology Studies*, The MIT Press, 2008.
 3. D. MacKenzie and J. Wajcman (eds.), *The Social Shaping of Technology*, The Open University Press, 1999.
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CHE-SE-3054: CHEMOINFORMATICS

(Credits: 04)

Learning Objectives: The primary objective of this course is to familiarize the students with the use of various computer software and information technology. The students are expected to learn different chemical search engines and utilize them for molecular modelling and structure elucidation with a final goal to compute NMR, IR, mass and other spectra that can be later compared with the experimental data. The course also provides sufficient information and hands on exercises on the use of cheminformatics, with a special emphasis on its application in modern drug discovery.

Learning Outcomes: On the successful completion of the course, the students should be able to explain, interpret and critically examine the utility of computers and software tools to solving chemistry related problems. Recognize, apply, compare and predict chemical structures, properties, and reactivity and; solve chemistry related problems.

Employ critical thinking and scientific reasoning to design and safely implement laboratory experiments and keep the records of the same.

Compile, interpret and analyze the qualitative/quantitative data and communicate the same in a scientific literature

Introduction to Chemoinformatics: History and evolution of chemoinformatics, Use of chemoinformatics, Prospects of chemoinformatics, Molecular Modelling and Structure elucidation.

Representation of molecules and chemical reactions: Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification.

Searching chemical structures: Full structure search, sub-structure search, basic ideas, similarity search, three dimensional search methods, basics of computation of physical and chemical data and structure descriptors, data visualization.

Applications: Prediction of Properties of Compounds; Linear Free Energy Relations; Quantitative Structure-Property Relations; Descriptor Analysis; Model Building; Modeling Toxicity; Structure-Spectra correlations; Prediction of NMR, IR and Mass spectra; Computer Assisted Structure elucidations; Computer Assisted Synthesis Design, Introduction to drug design; Target Identification and Validation; Lead Finding and Optimization; Analysis of HTS data; Virtual Screening; Design of Combinatorial Libraries; Ligand-Based and Structure Based Drug design; Application of Cheminformatics in Drug Design.

Hands-on Exercises

Recommended Books:

1. Andrew R. Leach & Valerie, J. Gillet (2007) *An introduction to Cheminformatics*. Springer: The Netherlands.
 2. Gasteiger, J. & Engel, T. (2003) *Cheminformatics: A text-book*. Wiley-VCH.
 3. Gupta, S. P. (2011) *QSAR & Molecular Modeling*. Anamaya Pub.: New Delhi.
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CHE-SE-3064: BUSINESS SKILLS FOR CHEMISTS

(Credits: 04)

Course Objective: To familiarize students with important concepts of business operations and intellectual rights as applied to chemical industry.

Learning outcome: students shall be able to explain and/or analyze the important steps of business operations, finance and intellectual property as applied to chemical industry.

Chemistry in Industry

Current challenges and opportunities for the chemistry-using industries, role of chemistry in

India and global economies.

Basics of Business and Management

Key business concepts: Business plans, market need, project management and routes to market. Management Functions and skills, principles of motivation, forms of business organization including partnerships and companies.

Marketing Skills

Understanding basics of marketing and marketing mix strategies with cases.

Human Resource Management (HRM) Skills

Managerial HRM functions viz. recruitment, training and development and compensation.

Financial Management Skills

An overview of financial and cost accounting with cases, managerial finance functions.

Intellectual Property Rights

Concept of intellectual property rights, patents.

Recommended books

1. <http://www.rsc.org/learn-chemistry/resources/business-skills-forchemists/OnlineCourse/>
 2. Philip Kotler, Keven Lane Keller Marketing Management 15th Ed., Pearson Education; Fifteenth edition (10 August 2017)
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CHE-SE-3074: INTELLECTUAL PROPERTY RIGHTS (IPR)

(Credits: 04)

***Course Objective:** In this era of liberalization and globalization, the perception about science and its practices has undergone dramatic change. The importance of protecting the scientific discoveries, with commercial potential or the intellectual property rights is being discussed at all levels – statutory, administrative, and judicial. With India ratifying the WTO agreement, it has become obligatory on its part to follow a minimum acceptable standard for protection and enforcement of intellectual property rights. The purpose of this course is to apprise the students about the multifaceted dimensions of this issue.*

***Learning Outcome:** After completing this course, students will have in-depth understanding about the importance and types of IPR. This course will also provide the clarity on the legal and economic aspects of the IP system.*

Introduction to Intellectual Property:

Historical Perspective, Different Types of IP, Importance of protecting IP.

Copyrights

Introduction, How to obtain, Differences from Patents.

Trade Marks

Introduction, How to obtain, Different types of marks – Collective marks, certification marks, service marks, Trade names, etc.

Differences from Designs.

Patents

Historical Perspective, Basic and associated right, WIPO, PCT system, Traditional Knowledge, Patents and Healthcare – balancing promoting innovation with public health,

Software patents and their importance for India.

Geographical Indications

Definition, rules for registration, prevention of illegal exploitation, importance to India.

Industrial Designs

Definition, How to obtain, features, International design registration.

Layout design of integrated circuits

Circuit Boards, Integrated Chips, Importance for electronic industry.

Trade Secrets

Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection.

Different International agreements

(a) World Trade Organization (WTO):

- (i) General Agreement on Tariffs & Trade (GATT), Trade Related Intellectual Property Rights (TRIPS) agreement
- (ii) General Agreement on Trade related Services (GATS)
- (iii) Madrid Protocol
- (iv) Berne Convention
- (v) Budapest Treaty

(b) Paris Convention

WIPO and TRIPS, IPR and Plant Breeders Rights, IPR and Biodiversity

IP Infringement issue and enforcement – Role of Judiciary, Role of law enforcement agencies – Police, Customs etc. Economic Value of Intellectual Property – Intangible assets and their valuation, Intellectual Property in the Indian Context – Various laws in India
Licensing and technology transfer.

Recommended Books:

1. N.K. Acharya: *Textbook on intellectual property rights*, Asia Law House (2001).
2. Manjula Guru & M.B. Rao, *Understanding Trips: Managing Knowledge in Developing Countries*, Sage Publications (2003).
3. P. Ganguli, *Intellectual Property Rights: Unleashing the Knowledge Economy*, Tata McGraw-Hill (2001).
4. Arthur Raphael Miller, Micheal H.Davis; *Intellectual Property: Patents, Trademarks and Copyright in a Nutshell*, West Group Publishers (2000).
5. Jayashree Watal, *Intellectual property rights in the WTO and developing countries*, Oxford University Press, Oxford.

CHE-SE-4014: ANALYTICAL CLINICAL BIOCHEMISTRY

(Credits: 04)

Course objective: *This course is intended to apprise students with various clinically relevant biomolecules, their structures and physiological roles. Students are also expected to learn the basics of analysis of pathological samples (blood and urine).*

Learning outcome: *Students will be able to identify various molecules relevant to a particular pathological condition and their estimation protocols.*

Basic understanding of the structures, properties and functions of carbohydrates, lipids and proteins:

Review of concepts studied in the core course.

Carbohydrates: Biological importance of carbohydrates, metabolism, cellular currency of energy (ATP), glycolysis, alcoholic and lactic acid fermentations, Krebs cycle, Isolation and characterization of polysaccharides.

Proteins: Classification, biological importance, primary and secondary, tertiary and quaternary structures of proteins: α -helix and β -pleated sheets, isolation, characterization, denaturation of proteins.

Enzymes: Nomenclature, characteristics, classification, active site, mechanism of enzyme action, stereospecificity of enzymes, effect of pH, temperature on enzyme activity, enzyme inhibitors, coenzymes and cofactors introduction to biocatalysis: importance in "Green Chemistry" and chemical industry.

Lipids: Classification, biological importance of triglycerides and phosphoglycerides and cholesterol, lipid membrane, liposomes and their biological functions and underlying applications. Lipoproteins. Properties, functions and biochemical functions of steroid hormones. Biochemistry of peptide hormones. *Structure of DNA* (Watson-Crick model) and RNA, genetic code, biological roles of DNA and RNA: replication, transcription and translation, introduction to gene therapy.

Biochemistry of disease: A diagnostic approach by blood/ urine analysis:

Blood: Composition and functions of blood, blood coagulation, blood collection and preservation of samples, anemia, regulation, estimation and interpretation of data for blood sugar, urea, creatinine, cholesterol and bilirubin.

Urine: Collection and preservation of samples, formation of urine, composition and estimation of constituents of normal and pathological urine.

Practicals:

Identification and estimation of the following:

1. Carbohydrates - qualitative and quantitative analysis.
2. Lipids - qualitative and quantitative analysis.
3. Determination of the iodine number of oil.
4. Determination of the saponification number of oil.
5. Detection of cholesterol using Liebermann- Burchard reaction.
6. Isolation of protein.
7. Determination of concentration of protein by the Biuret reaction.
8. Determination of nucleic acid concentration.
9. Separation of nucleic acids.

Recommended Books:

1. David L. Nelson and Michael M. Cox: Lehninger Principles of Biochemistry
2. T.G. Cooper: Tool of Biochemistry.
3. Keith Wilson and John Walker: Practical Biochemistry.
4. Alan H Gowenlock: Varley's Practical Clinical Biochemistry.
5. Thomas M. Devlin: Textbook of Biochemistry.
6. Jeremy M. Berg, John L Tymoczko, Lubert Stryer: Biochemistry.
7. G. P. Talwar and M Srivastava: Textbook of Biochemistry and Human Biology.
8. O. Mikes, R.A. Chalmers: Laboratory Handbook of Chromatographic Methods.

CHE-SE-4024: GREEN METHODS IN CHEMISTRY

(Credits: 04)

Course Objectives: This course introduces students to the utilization of green chemistry from industrial perspective and provides exposure to methods by which environmental problems are evaluated and designing of sustainable solutions.

Learning Outcome: Students shall be able to describe and evaluate chemical products and

processes from environmental perspective, define and propose sustainable solutions and critically assess the methods for waste reduction and recycling.

Tools of Green chemistry, Twelve principles of Green Chemistry, with examples.

The following Real world Cases in Green Chemistry should be discussed:

- 1 A green synthesis of ibuprofen which creates less waste and fewer byproducts (Atom economy).
- 2 Surfactants for Carbon Dioxide – replacing smog producing and ozone depleting solvents with CO₂ for precision cleaning and dry cleaning of garments.
- 3 Environmentally safe antifoulant.
- 4 CO₂ as an environmentally friendly blowing agent for the polystyrene foam sheet packaging market.
- 5 Using a catalyst to improve the delignifying (bleaching) activity of hydrogen peroxide.
- 6 A new generation of environmentally advanced preservative: getting the chromium and arsenic out of pressure treated wood.
7. Rightfit pigment: synthetic azopigments to replace toxic organic and inorganic pigments.
- 8 Development of a fully recyclable carpet: cradle to cradle carpeting.

Recommended Books:

1. Manahan S.E. (2005) Environmental Chemistry, CRC Press
2. Miller, G.T. (2006) Environmental Science 11th edition. Brooks/Cole
3. Mishra, A. (2005) Environmental Studies. Selective and Scientific Books, New

CHE-SE-4034: PHARMACEUTICAL CHEMISTRY

(Credits: 04)

Course Objective: This primary objective of this course is to introduce students to the fundamentals of drug design and development process, drugs for various diseases available in market, their mode of action and side effects. Students are expected to learn the biosynthetic procedures of various bio-relevant small molecules.

Learning Outcome: Students will be able to appreciate the drug development process, identify various small molecules used for treatments different ailments and other physiological processes.

Drugs & Pharmaceuticals:

Drug discovery, design and development; basic retrosynthetic approach, synthesis of the representative drugs of the following classes: analgesics, antipyretic, anti-inflammatory (aspirin, paracetamol, ibuprofen), antibiotics (chloramphenicol), antibacterial and antifungal (sulphonamides, sulphamethoxazol, sulphacetamide, trimethoprim), antiviral (acyclovir), drugs effecting central nervous system (phenobarbital, diazepam), cardiovascular (glyceryl trinitrate), antilaprosy (dapson), HIV-AIDS related drugs (AZT- Zidovudine).

Fermentation:

Aerobic and anaerobic fermentation, production of (i) ethanol and citric acid, (ii) antibiotics (penicillin, cephalosporin, chloromycetin and streptomycin), (iii) lysine, glutamic acid, vitamin B₂, vitamin B₁₂ and vitamin C.

Practicals:

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

Recommended Books:

1. Graham L. Patrick: *An Introduction to Medicinal Chemistry*, Oxford University Press, UK.
2. Gareth Thomas: *Fundamentals of Medicinal Chemistry*, Wiley.

3. Hakishan, V.K. Kapoor: *Medicinal and Pharmaceutical Chemistry*, Vallabh Prakashan, Pitampura, New Delhi.

4. William O. Foye, Thomas L., Lemke, David A. William: *Principles of Medicinal Chemistry*, B.I. Waverly Pvt. Ltd. New Delhi.

CHE-SE-4044: CHEMISTRY OF COSMETICS & PERFUMES

(Credits: 04)

60 Lectures

Course Objective: This course intends to apprise students about the chemical knowledge related to some of the commonly used cosmetics. Laboratory experiments for preparation of talcum powder, shampoo etc. are included to give hands on experience.

Learning Outcome: Students will learn about the preparation and chemistry involved with the production different cosmetic. This may encourage students to take up entry level jobs at cosmetics industry or venture into commercial production of cosmetics as an entrepreneur.

A general study including preparation and uses of the following: Hair dye, hair spray, shampoo, suntan lotions, face powder, lipsticks, talcum powder, nail enamel, creams (cold, vanishing and shaving creams), antiperspirants and artificial flavours. Essential oils and their importance in cosmetic industries with reference to Eugenol, Geraniol, sandalwood oil, eucalyptus, rose oil, 2-phenyl ethyl alcohol, Jasmone, Civetone, Muscone.

Practicals

1. Preparation of talcum powder.
2. Preparation of shampoo.
3. Preparation of enamels.
4. Preparation of hair remover.
5. Preparation of face cream.
6. Preparation of nail polish and nail polish remover.

Recommended Books:

1. E. Stocchi: *Industrial Chemistry*, Vol -I, Ellis Horwood Ltd. UK.
 2. P.C. Jain, M. Jain: *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.
 3. B.K. Sharma: *Industrial Chemistry*, Goel Publishing House, Meerut.
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CHE-SE-4054: PESTICIDE CHEMISTRY

(Credits: 04)

Course Objective: This is a brief and introductory course on pesticides, through which the students will be introduced to various classes of pesticides, their synthesis, applications and possible hazards of their uses.

Learning Outcome: Students will be able to explain or describe and critically examine different types of pesticides, their activity/toxicity and their applications and the need for the search of an alternative based on natural products.

Definition of pesticides, general introduction to pesticides (natural and synthetic), benefits and adverse effects of pesticides. Classification, mode of action, toxicity and methods of pesticides residue analysis. Synthesis and technical manufacture and uses of representative pesticides in the following classes: Organochlorines (DDT, Gammexene); organophosphate (Malathion, Parathion); Carbamates (Carbofuran and carbaryl); Quinones (Chloranil), Anilides (Alachlor and Butachlor)

Practicals:

1. To calculate acidity/alkalinity in given sample of pesticides formulations as per BIS specifications.

2. Preparation of simple organophosphates, phosphonates and thiophosphates.

Recommended Book:

1. R. Cremllyn: Pesticides, Preparation and Mode of Action, John Wiley & Sons, New York, 1978
 2. RPBateman, Pesticide Applications, AAB Press, 2004
 3. Principles of Pesticide chemistry: S K Handa, Ed. by Agrobios (India), 2008
 4. Pesticide Science & Biotechnology: R Greenhalgh and T R Robers, IUPAC, Blackwell Scientific Publications, 1987
 5. The Chemical Process Industries: D N Shreve
 6. Pesticide Chemistry : G Matolesy, M. Nadasy, V. Andriska, Elsevier Sc. Publisher, USA, 1988
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CHE-SE-4064: FUEL CHEMISTRY

(Credits: 04)

Course Objectives: This course discusses about the chemistry of various sources of energy. Students are expected to learn about the composition of coal and petroleum products, their extraction, purification methods and usage. A section also covers classification and applications of natural and synthetic lubricants. Students will also learn about the determination and significance of various industrially relevant physical parameters for different fuels and lubricants.

Learning Outcomes: At the end of this course students will learn about the classes of renewable and non-renewable energy sources. Students will learn about the composition of coal and crude petroleum, their classification, isolation of coal and petroleum products and their usage in various industries. They will also learn to determine industrially significant physical parameters for fuels and lubricants.

Fuel Chemistry

Review of energy sources (renewable and non-renewable). Classification of fuels and their calorific value.

Coal: Uses of coal (fuel and nonfuel) in various industries, its composition, carbonization of coal. Coal gas, producer gas and water gas—composition and uses. Fractionation of coal tar, uses of coal tar bases chemicals, requisites of a good metallurgical coke, Coal gasification (Hydro gasification and Catalytic gasification), Coal liquefaction and Solvent Refining.

Petroleum and Petrochemical Industry: Composition of crude petroleum, Refining and different types of petroleum products and their applications.

Fractional Distillation (Principle and process), Cracking (Thermal and catalytic cracking), Reforming Petroleum and non-petroleum fuels (LPG, CNG, LNG, bio-gas, fuels derived from biomass), fuel from waste, synthetic fuels (gaseous and liquids), clean fuels.

Petrochemicals: Vinyl acetate, Propylene oxide, Isoprene, Butadiene, Toluene and its derivatives Xylene.

Lubricants: Classification of lubricants, lubricating oils (conducting and non-conducting) Solid and semisolid lubricants, synthetic lubricants.

Properties of lubricants (viscosity index, cloud point, pore point) and their determination.

Recommended Books:

1. E. Stocchi: *Industrial Chemistry*, Vol -I, Ellis Horwood Ltd. UK.
2. P.C. Jain, M. Jain: *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.
3. B.K. Sharma: *Industrial Chemistry*, Goel Publishing House, Meerut.